

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
 Data File : BP007163.D
 Acq On : 24 Sep 2021 17:41
 Operator : CG/JU
 Sample : M3875-15
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20882

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007163.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.364	42	47	60	rBV	399270	1080385	4.74%	0.241%
2	3.787	93	119	123	rBV	2142414	5587689	24.53%	1.248%
3	3.840	124	128	132	rVB2	1341749	2408750	10.58%	0.538%
4	4.169	158	184	186	rBV	866814	3972037	17.44%	0.887%
5	4.216	186	192	199	rBV	2984136	4320076	18.97%	0.965%
6	4.334	207	212	217	rBV	1975690	2762114	12.13%	0.617%
7	4.405	217	224	230	rVB	11405715	19209664	84.34%	4.289%
8	4.516	237	243	253	rBV2	2843484	4554375	20.00%	1.017%
9	4.893	285	307	313	rBV3	1721349	5886324	25.84%	1.314%
10	5.005	321	326	331	rVB	3004391	4965648	21.80%	1.109%
11	5.105	338	343	346	rVB	582250	989101	4.34%	0.221%
12	5.469	390	405	410	rBV	4425610	7368498	32.35%	1.645%
13	6.622	565	601	602	rBV3	1246008	7310534	32.10%	1.632%
14	7.028	656	670	672	rBV	1176894	2546881	11.18%	0.569%
15	7.069	672	677	679	rBV	2647143	4144459	18.20%	0.925%
16	7.887	810	816	823	rVB	895218	1512201	6.64%	0.338%
17	7.963	823	829	836	rBV3	403142	817926	3.59%	0.183%
18	8.110	848	854	862	rBV3	1265703	2198167	9.65%	0.491%
19	8.546	915	928	935	rVB4	588460	1499572	6.58%	0.335%
20	8.657	939	947	961	rBV	1816115	3205577	14.07%	0.716%
21	8.934	982	994	1000	rVV	1562529	3258883	14.31%	0.728%
22	9.016	1001	1008	1010	rVV	560813	925854	4.06%	0.207%
23	9.051	1010	1014	1023	rVV	2542580	4318478	18.96%	0.964%
24	9.410	1064	1075	1089	rBV	4203417	9606725	42.18%	2.145%
25	9.993	1165	1174	1177	rVV3	318571	850952	3.74%	0.190%
26	10.051	1179	1184	1187	rVV	575513	1336751	5.87%	0.298%
27	10.093	1187	1191	1199	rVV2	619622	1290213	5.66%	0.288%
28	10.328	1223	1231	1235	rBV	451608	832941	3.66%	0.186%
29	10.687	1283	1292	1297	rVV	1149251	2049651	9.00%	0.458%
30	10.987	1337	1343	1348	rBV2	940730	2194624	9.64%	0.490%
31	11.057	1349	1355	1360	rBV	2435831	4521058	19.85%	1.010%
32	11.251	1375	1388	1394	rVB3	2261918	9346481	41.04%	2.087%
33	11.351	1398	1405	1408	rVV2	935534	1986921	8.72%	0.444%
34	11.445	1408	1421	1430	rVV2	3266371	12985001	57.01%	2.899%
35	11.522	1430	1434	1439	rVV2	428657	960059	4.22%	0.214%
36	11.704	1441	1465	1472	rVV6	3103353	18140435	79.65%	4.051%

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Integrator: RTE

Smoothing : ON

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Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.769	1472	1476	1481	rVV3	1810975	4282118	18.80%	0.956%
38	11.840	1481	1488	1493	rVV3	2799472	6443081	28.29%	1.439%
39	11.910	1494	1500	1505	rVB3	574028	1114898	4.89%	0.249%
40	11.975	1505	1511	1513	rBV	576752	876837	3.85%	0.196%
41	12.004	1513	1516	1520	rVV	1027489	1492565	6.55%	0.333%
42	12.051	1520	1524	1528	rVB	659395	921082	4.04%	0.206%
43	12.610	1604	1619	1627	rVV	2985800	8921744	39.17%	1.992%
44	12.863	1657	1662	1667	rVB2	608422	976203	4.29%	0.218%
45	13.145	1704	1710	1719	rBV	6317038	9379549	41.18%	2.094%
46	13.645	1790	1795	1798	rBV	1404075	2288111	10.05%	0.511%
47	13.692	1800	1803	1806	rVV2	1033965	1622341	7.12%	0.362%
48	13.739	1806	1811	1815	rVV3	2098252	3823359	16.79%	0.854%
49	13.787	1815	1819	1827	rVV3	1336698	2573211	11.30%	0.575%
50	13.863	1827	1832	1838	rVB2	1000155	1713164	7.52%	0.383%
51	13.987	1848	1853	1864	rVB3	509402	974487	4.28%	0.218%
52	14.175	1879	1885	1890	rBV	6118321	8973397	39.40%	2.004%
53	14.445	1922	1931	1932	rBV2	1391799	2746640	12.06%	0.613%
54	14.486	1932	1938	1943	rBV	10256143	22776380	100.00%	5.086%
55	14.681	1966	1971	1973	rBV	1983809	2814590	12.36%	0.628%
56	14.728	1973	1979	1983	rVV2	2526619	6647937	29.19%	1.484%
57	14.781	1983	1988	1993	rVB2	4033723	7345145	32.25%	1.640%
58	14.892	2003	2007	2011	rBV	752260	946887	4.16%	0.211%
59	15.004	2016	2026	2033	rVV	4545800	10170032	44.65%	2.271%
60	15.081	2034	2039	2049	rVV4	912703	2568613	11.28%	0.574%
61	15.175	2049	2055	2062	rVB	9776043	15318576	67.26%	3.421%
62	15.422	2092	2097	2100	rBV2	700570	1038779	4.56%	0.232%
63	15.881	2167	2175	2179	rBV	3385726	5681322	24.94%	1.269%
64	16.016	2193	2198	2203	rBV	4622204	6806870	29.89%	1.520%
65	16.069	2203	2207	2218	rVB	4327531	6485008	28.47%	1.448%
66	16.163	2218	2223	2230	rBV3	495188	876107	3.85%	0.196%
67	16.292	2239	2245	2251	rVB	7290152	10568392	46.40%	2.360%
68	16.410	2258	2265	2281	rBV	5341318	12499011	54.88%	2.791%
69	16.686	2308	2312	2319	rVB2	541230	910446	4.00%	0.203%
70	17.033	2366	2371	2375	rBV2	645900	890785	3.91%	0.199%
71	17.210	2397	2401	2406	rBV	1012892	1314676	5.77%	0.294%
72	17.269	2406	2411	2416	rVB	2001003	2764897	12.14%	0.617%
73	17.657	2471	2477	2482	rVV	1743301	2545230	11.17%	0.568%
74	17.822	2501	2505	2511	rVB	1859604	2313408	10.16%	0.517%
75	17.886	2512	2516	2523	rBV	387029	866281	3.80%	0.193%
76	18.092	2537	2551	2558	rVV3	1833189	7980681	35.04%	1.782%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
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77	18.169	2559	2564	2569	rVV	3399910	5732118	25.17%	1.280%
78	18.245	2569	2577	2587	rVB	2855077	8909245	39.12%	1.989%
79	18.380	2589	2600	2606	rBV	8727896	21488588	94.35%	4.798%
80	18.433	2606	2609	2614	rVB	2789541	3240683	14.23%	0.724%
81	18.545	2623	2628	2637	rVB	572706	1344377	5.90%	0.300%
82	19.057	2711	2715	2721	rBV2	1464129	1926701	8.46%	0.430%
83	19.274	2748	2752	2755	rBV2	781271	1159532	5.09%	0.259%
84	19.392	2767	2772	2780	rBV4	1560922	2347341	10.31%	0.524%
85	19.686	2818	2822	2827	rBV3	562337	892704	3.92%	0.199%
86	19.827	2839	2846	2850	rBV	9869739	12530076	55.01%	2.798%
87	20.004	2872	2876	2882	rVB	3579644	4158684	18.26%	0.929%
88	20.174	2901	2905	2916	rVB2	1063463	2771479	12.17%	0.619%
89	20.504	2958	2961	2967	rVB	1299898	1694683	7.44%	0.378%
90	20.569	2968	2972	2975	rBV	700814	916332	4.02%	0.205%
91	21.286	3091	3094	3100	rVB	2856715	3294069	14.46%	0.736%
92	21.351	3101	3105	3108	rBV	2284137	3374279	14.81%	0.753%
93	21.551	3134	3139	3145	rBV	1307140	2586069	11.35%	0.577%
94	21.745	3168	3172	3177	rVB	969157	1159835	5.09%	0.259%
95	21.827	3182	3186	3197	rVB2	2185483	3056357	13.42%	0.682%
96	22.239	3252	3256	3264	rVB3	1568547	3058283	13.43%	0.683%
97	22.310	3265	3268	3275	rVB2	1433079	2247378	9.87%	0.502%
98	22.604	3313	3318	3331	rVB2	1617871	3056453	13.42%	0.682%
99	23.033	3386	3391	3398	rVB	1012524	2033835	8.93%	0.454%
100	23.768	3513	3516	3528	rVB4	1097581	2665453	11.70%	0.595%

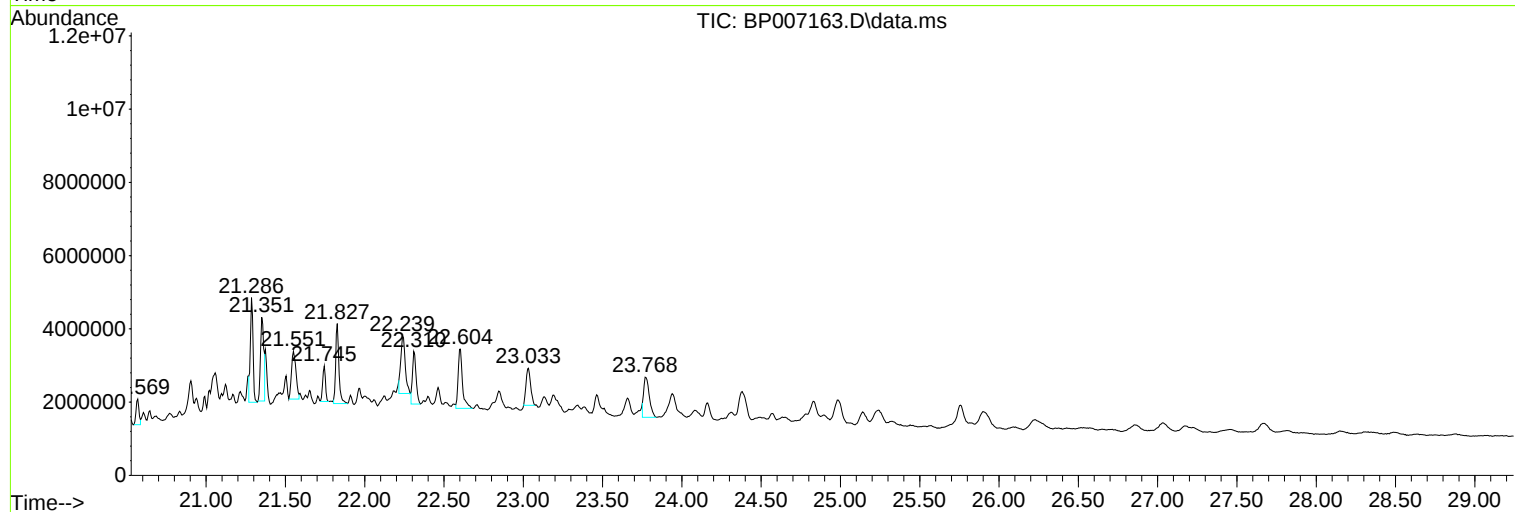
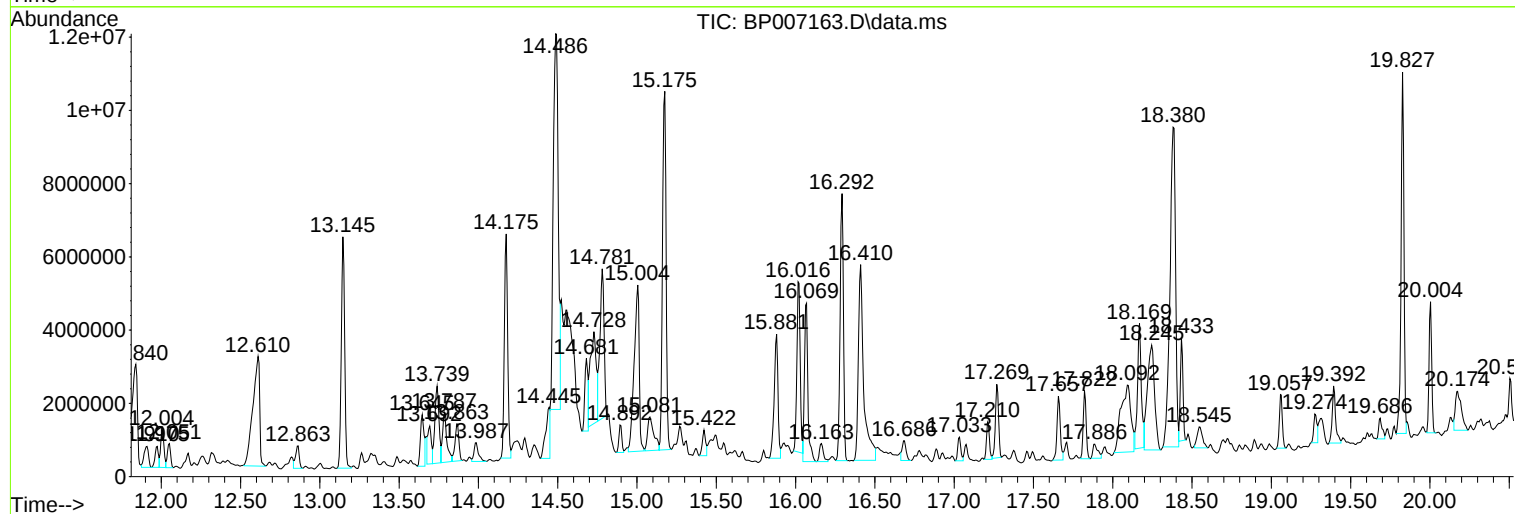
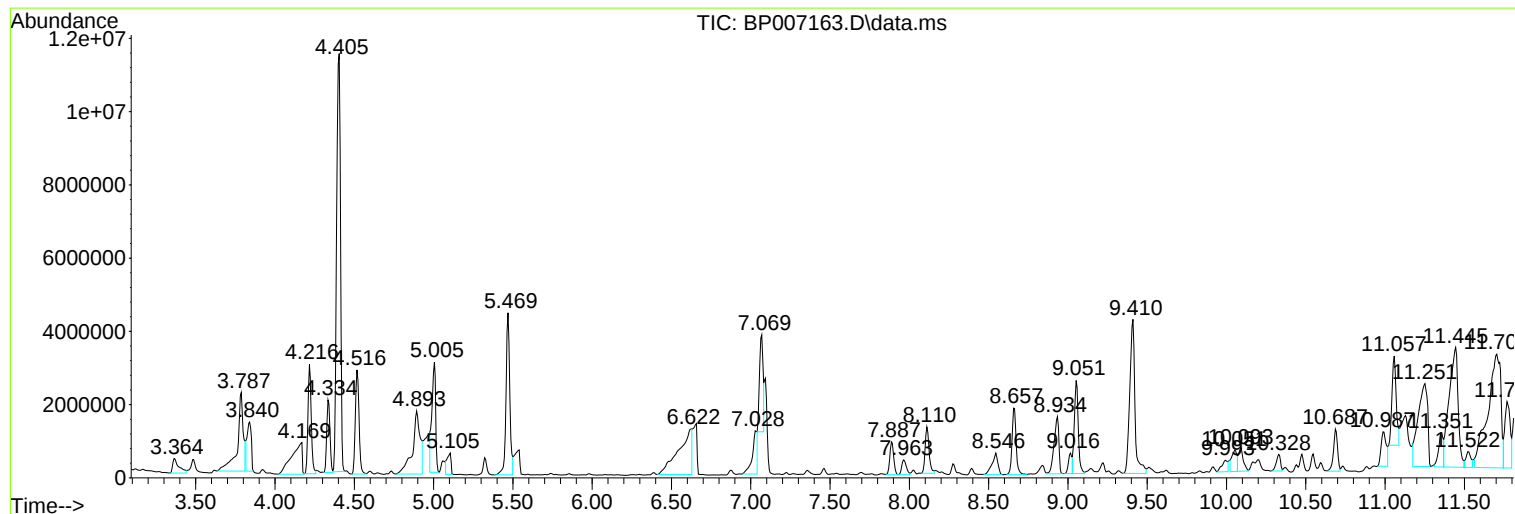
Sum of corrected areas: 447842399

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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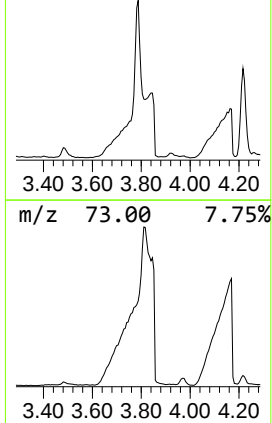
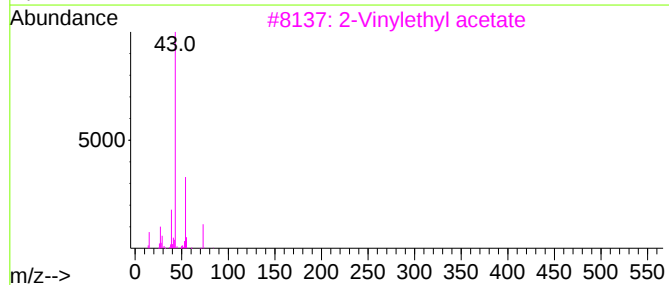
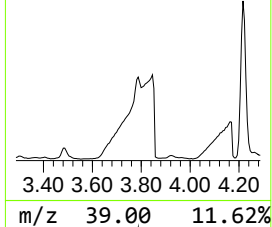
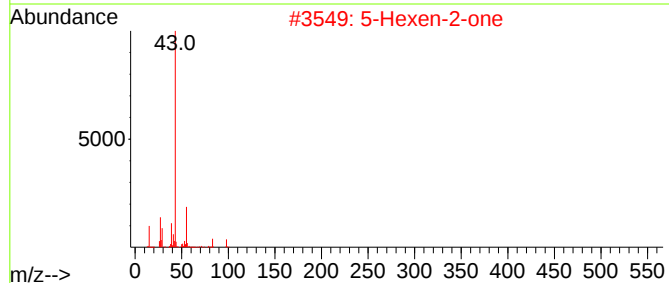
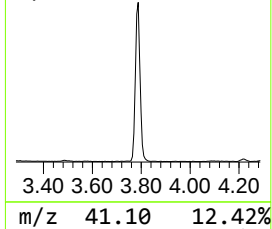
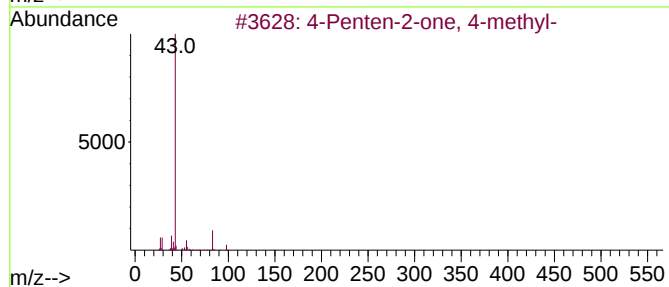
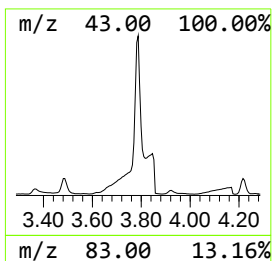
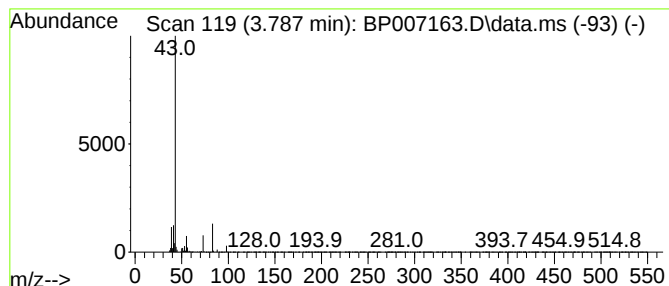
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Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.787	73.90 ng	5587690	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	50
2			5-Hexen-2-one	98	C6H10O	000109-49-9	38
3			2-Vinylethyl acetate	114	C6H10O2	001576-84-7	28
4			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	12
5			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	10



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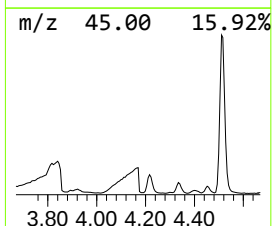
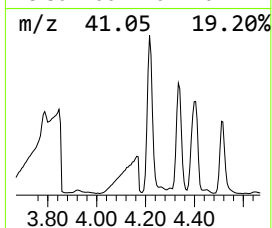
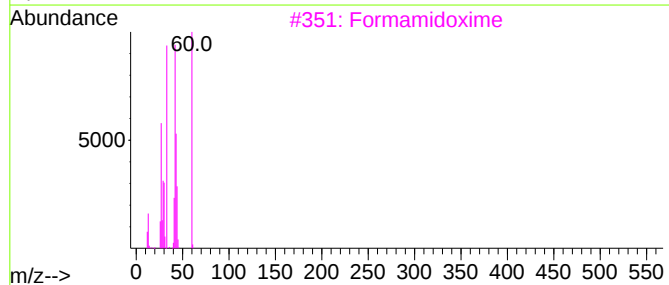
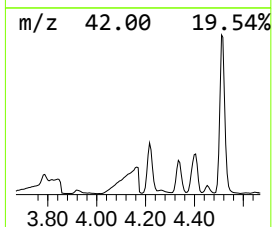
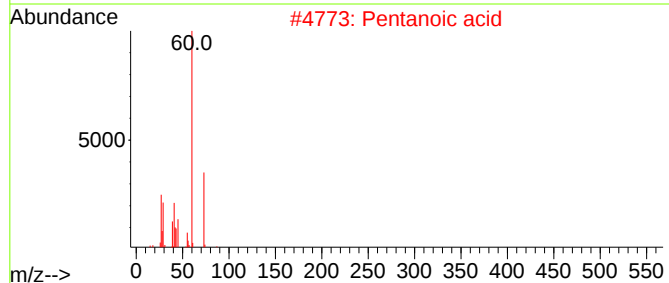
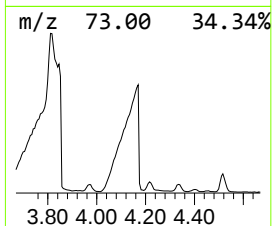
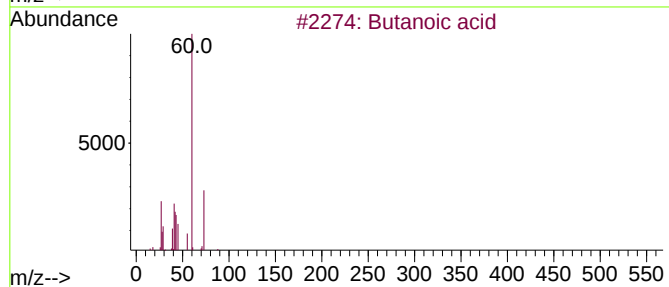
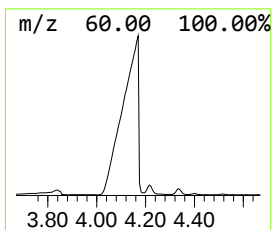
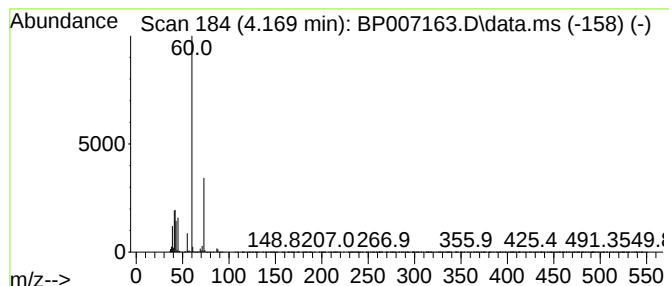
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.169	52.53 ng	3972040	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	91
2			Pentanoic acid	102	C5H10O2	000109-52-4	72
3			Formamidoxime	60	CH4N2O	000624-82-8	9
4			4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9
5			Hexanoic acid	116	C6H12O2	000142-62-1	9



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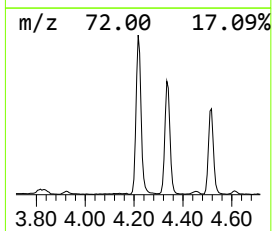
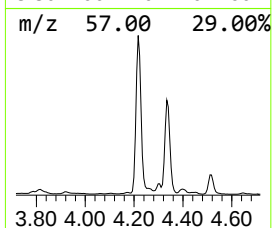
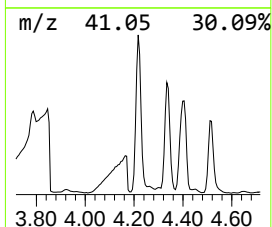
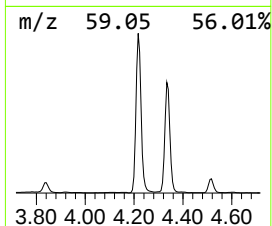
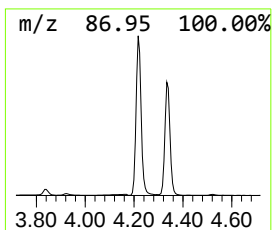
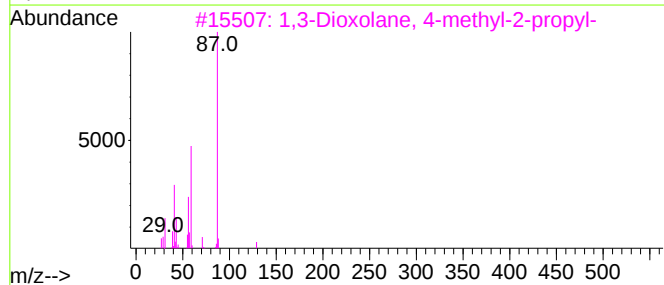
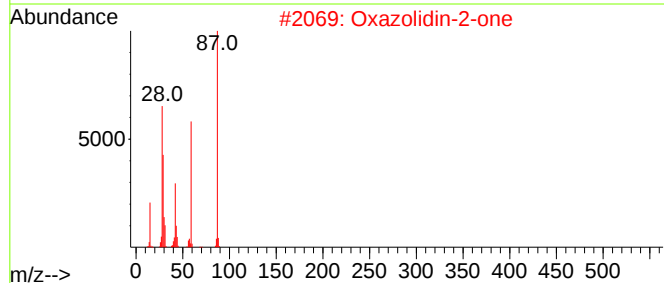
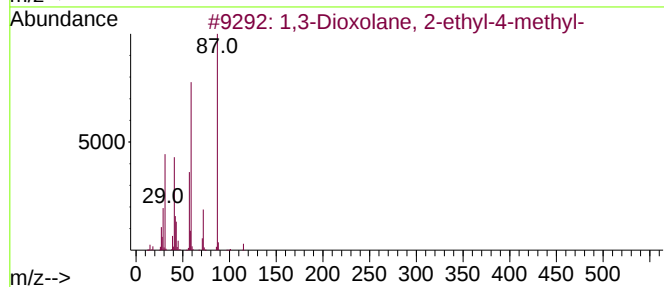
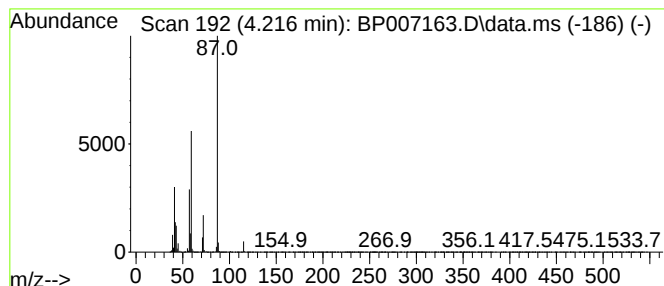
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.216	57.14 ng	4320080	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
4			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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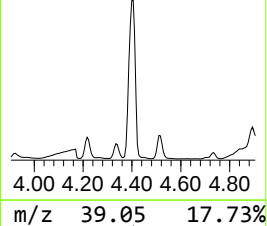
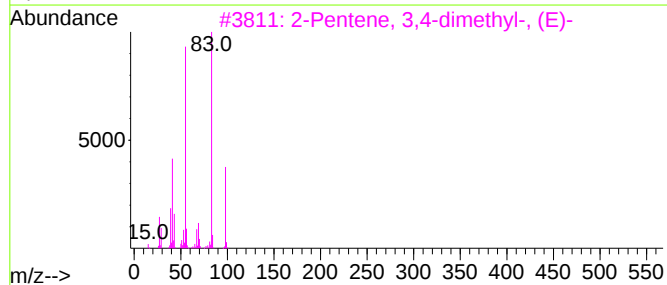
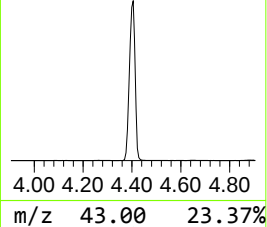
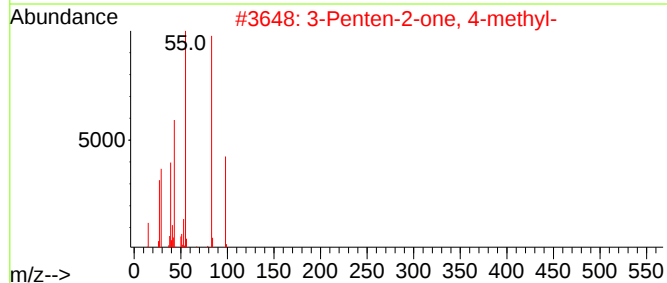
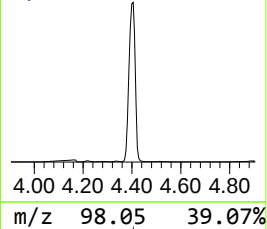
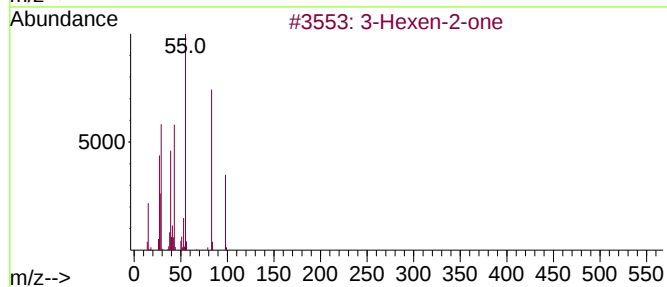
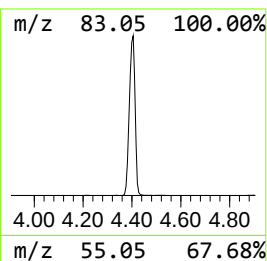
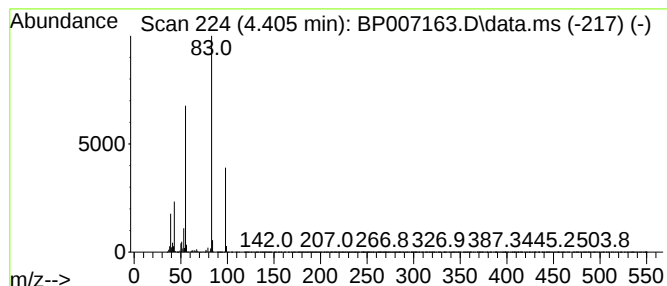
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Hexen-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.405	254.06 ng	19209700	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
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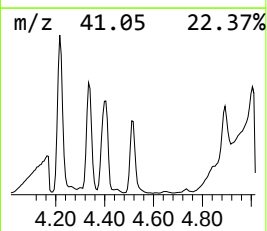
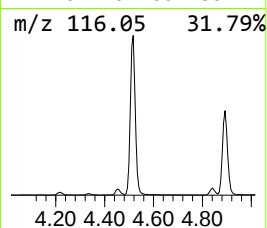
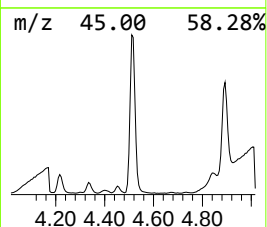
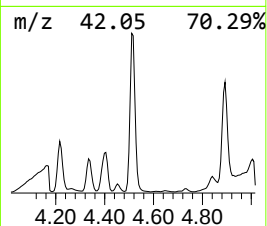
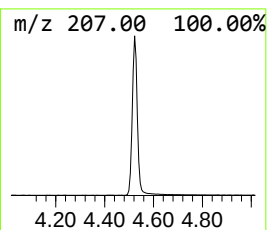
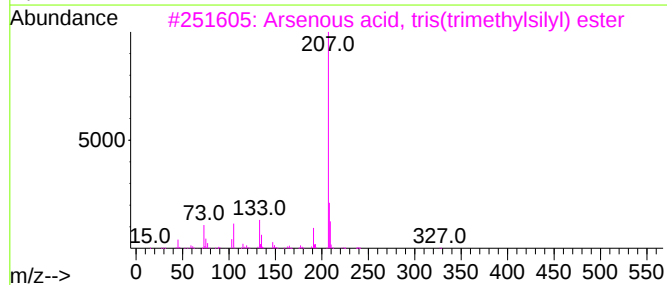
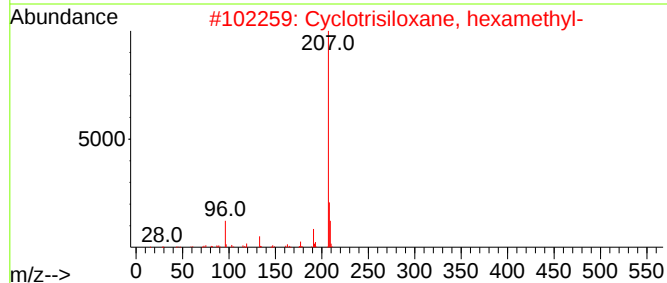
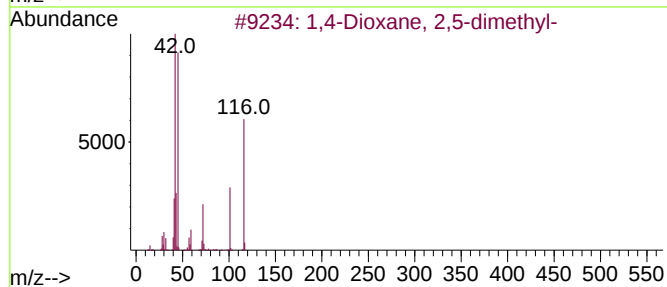
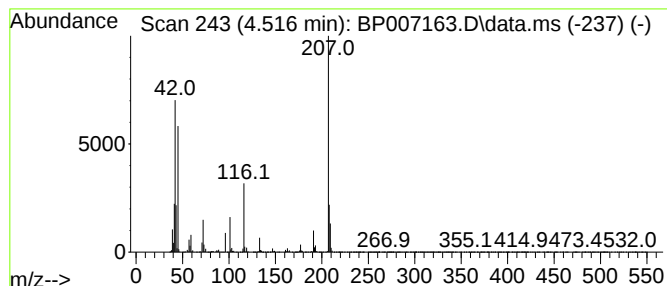
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Dioxane, 2,5-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.516	60.23 ng	4554380	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dioxane, 2,5-dimethyl-	116	C6H12O2	015176-21-3	89
2			Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	53
3			Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	47
4			4-Quinolinecarboxylic acid, 2-ch...	207	C10H6ClNO2	005467-57-2	33
5			4(15)-Selinene-11,12-diol	238	C15H26O2	073035-82-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
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Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

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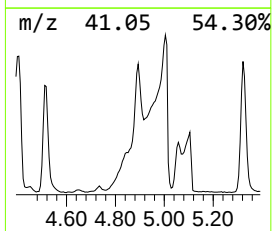
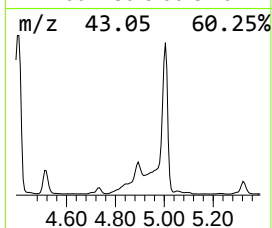
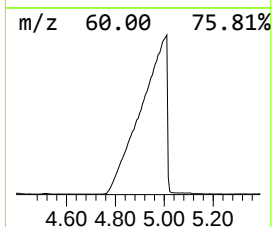
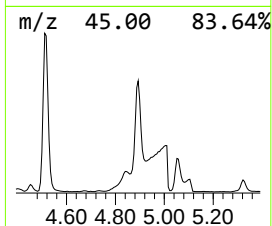
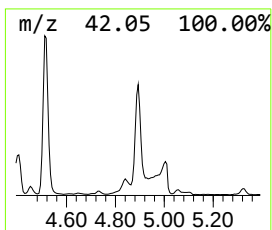
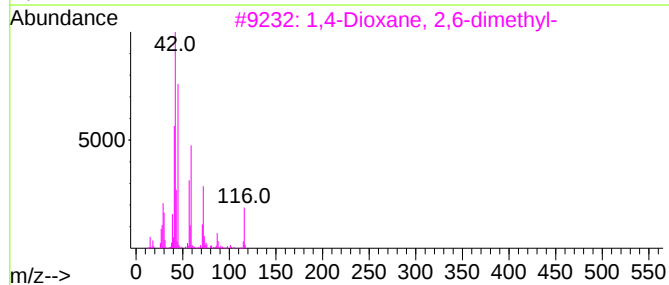
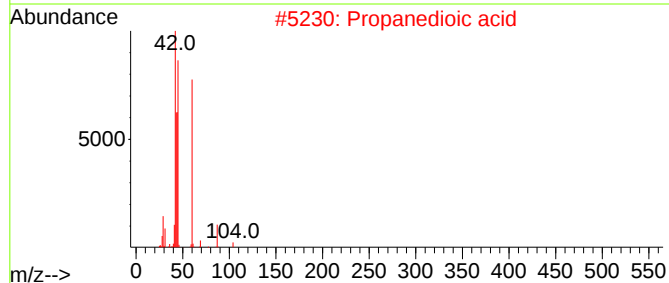
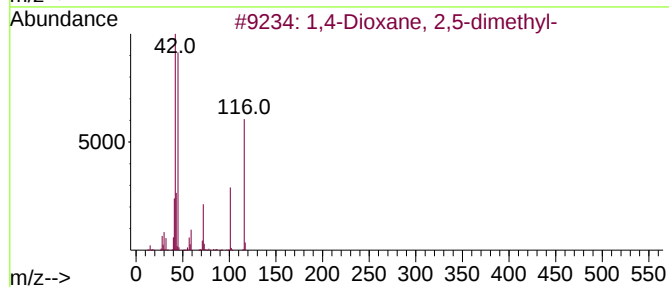
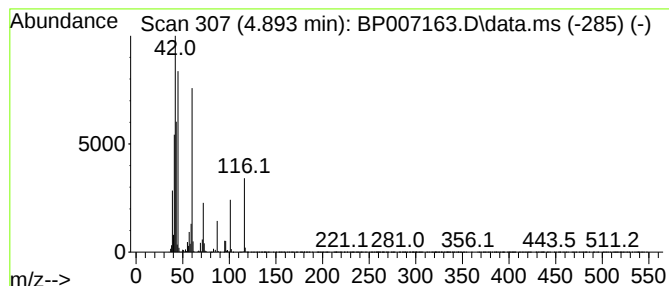
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Propanedioic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	77.85 ng	5886320	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dioxane, 2,5-dimethyl-	116	C6H12O2	015176-21-3	70
2			Propanedioic acid	104	C3H4O4	000141-82-2	59
3			1,4-Dioxane, 2,6-dimethyl-	116	C6H12O2	010138-17-7	47
4			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	43
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
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Sample : M3875-15
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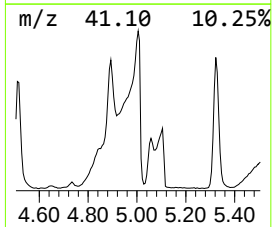
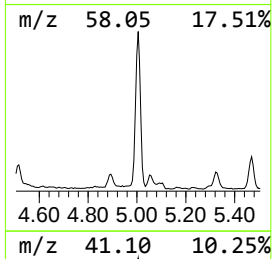
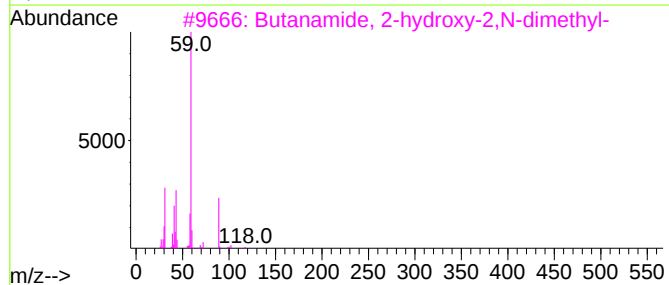
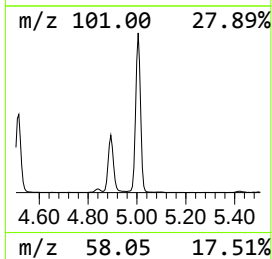
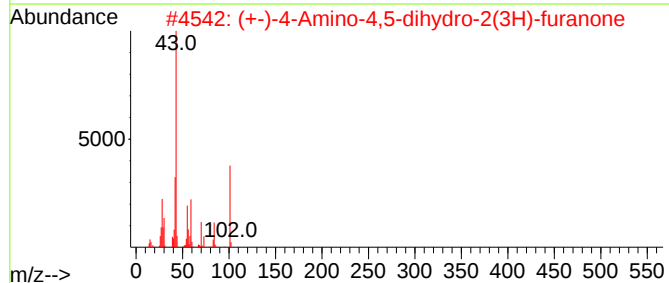
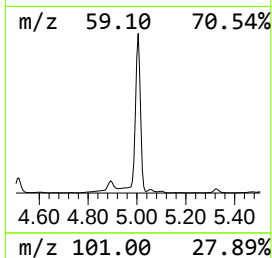
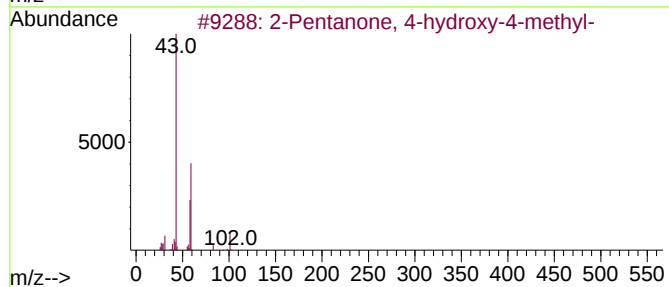
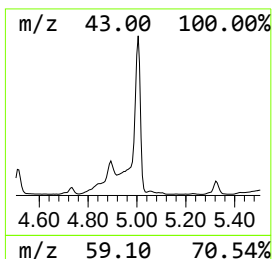
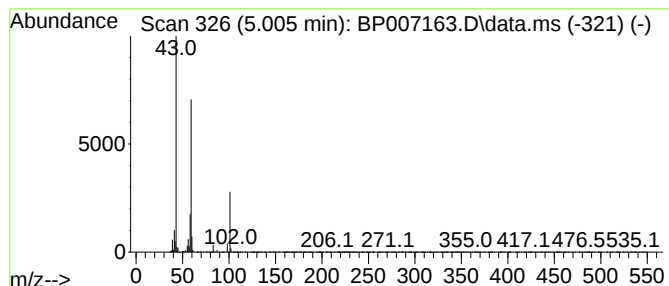
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.005	65.67 ng	4965650	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
3			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	23
4			Formamide, N-formyl-N-methyl-	87	C3H5NO2	018197-25-6	9
5			Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
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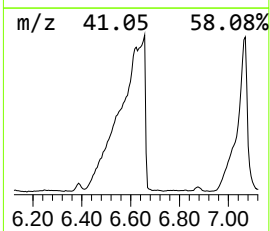
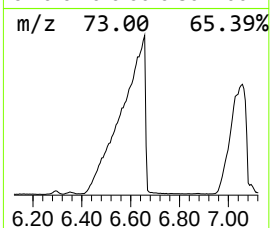
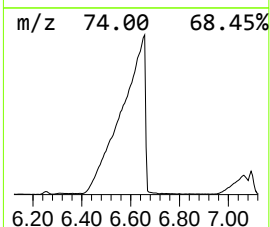
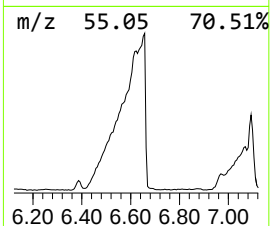
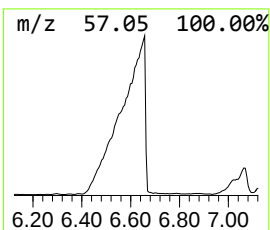
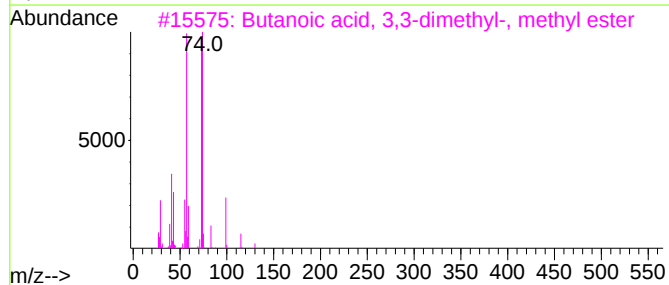
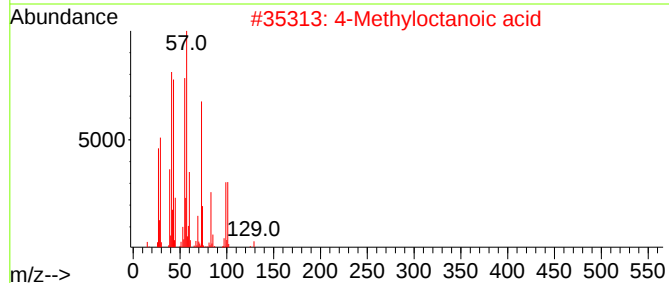
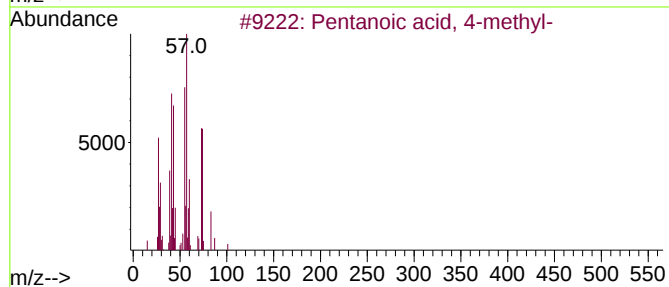
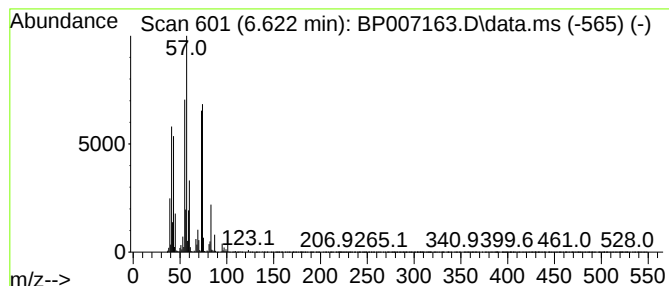
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentanoic acid, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.622	96.69 ng	7310530	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	90
2			4-Methyloctanoic acid	158	C9H18O2	054947-74-9	42
3			Butanoic acid, 3,3-dimethyl-, me...	130	C7H14O2	010250-48-3	38
4			Hexanoic acid, 5-methyl-, methyl...	144	C8H16O2	002177-83-5	25
5			1,2,3,4-Tetradecanetetrol, [2R-(...	262	C14H30O4	136953-04-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
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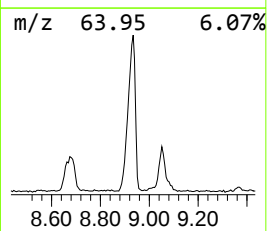
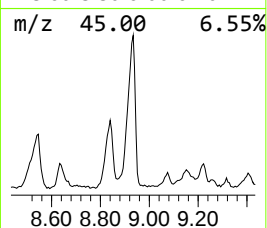
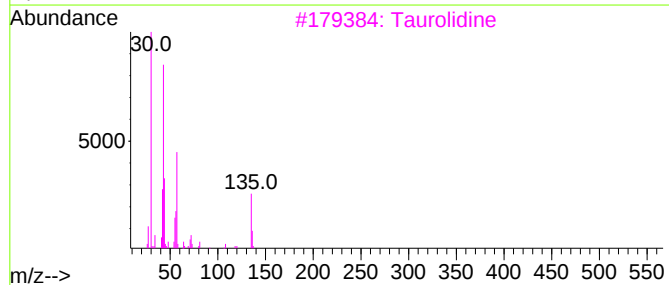
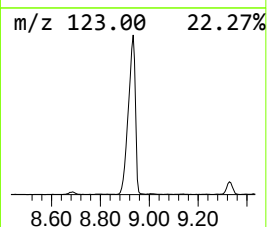
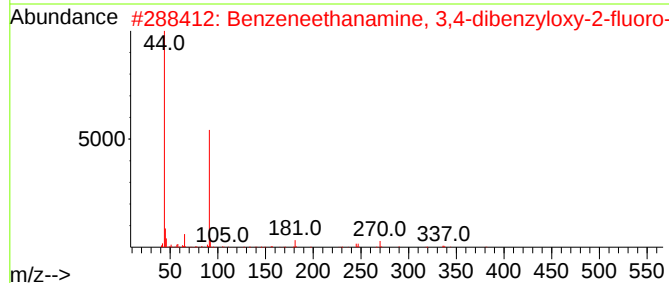
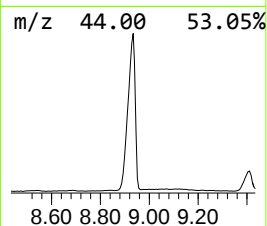
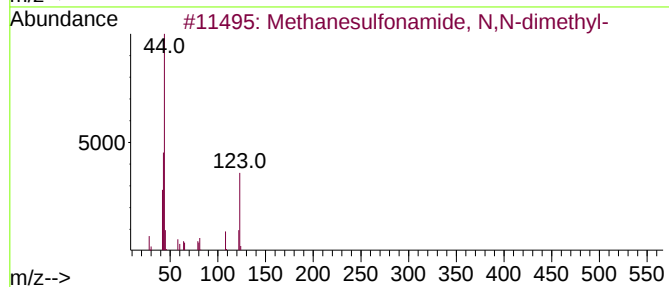
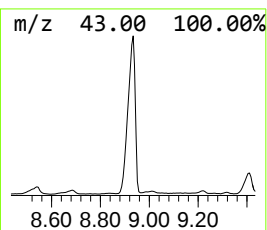
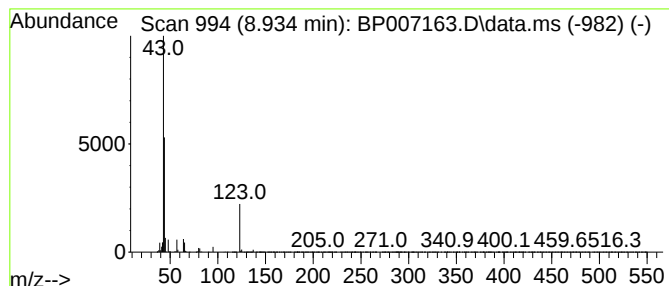
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown8.934 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.934	43.10 ng	3258880	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanesulfonamide, N,N-dimethyl-	123	C3H9NO2S	000918-05-8	9
2			Benzeneethanamine, 3,4-dibenzylo...	381	C23H24FNO3	115562-23-7	4
3			Taurolidine	284	C7H16N4O4S2	019388-87-5	4
4			8-(2-Acetyloxiran-2-yl)-6,6-dime...	236	C14H20O3	091186-38-8	4
5			Chloroacetic acid, propyl ester	136	C5H9ClO2	005396-24-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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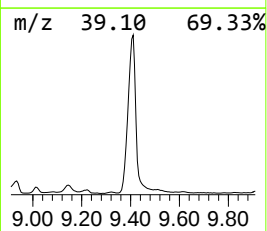
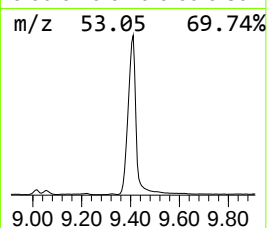
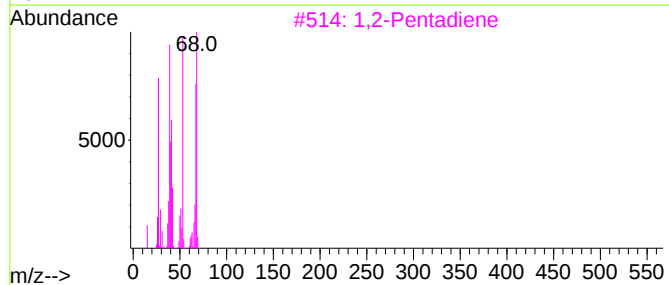
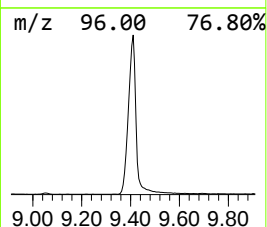
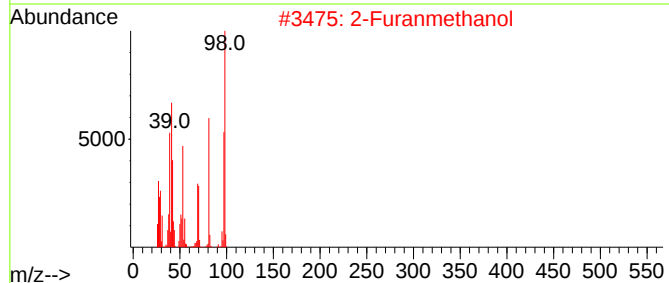
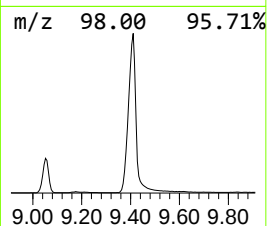
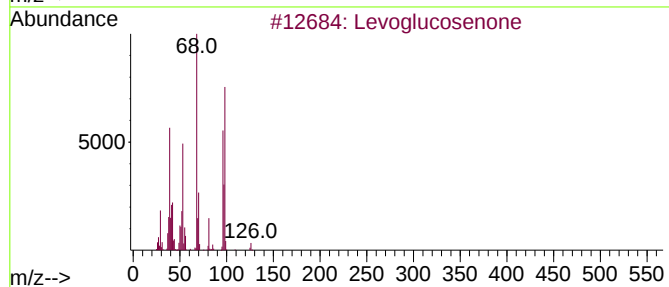
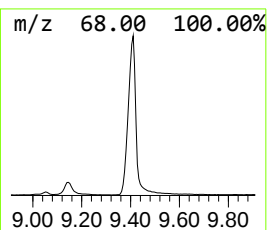
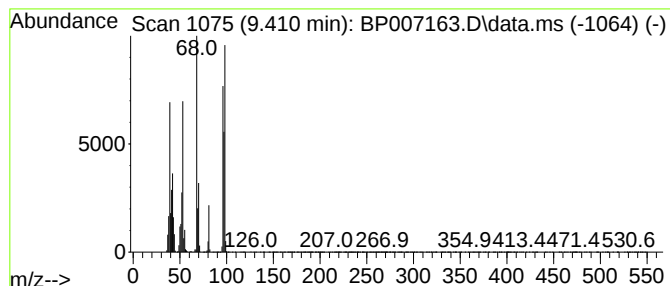
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Levoglucosenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	93.74 ng	9606730	Naphthalene-d8	10.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Levoglucosenone	126	C6H6O3	037112-31-5	64
2			2-Furanmethanol	98	C5H6O2	000098-00-0	53
3			1,2-Pentadiene	68	C5H8	000591-95-7	50
4			2,3-Pentadiene	68	C5H8	000591-96-8	41
5			2(3H)-Furanone, dihydro-3-methyl...	98	C5H6O2	000547-65-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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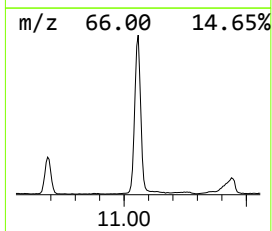
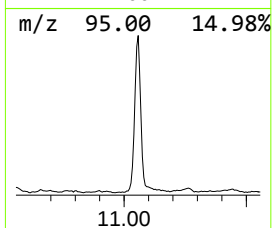
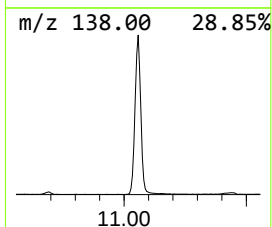
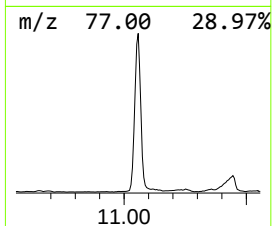
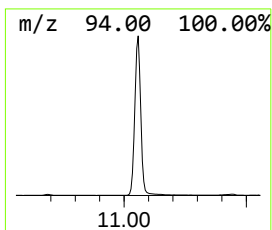
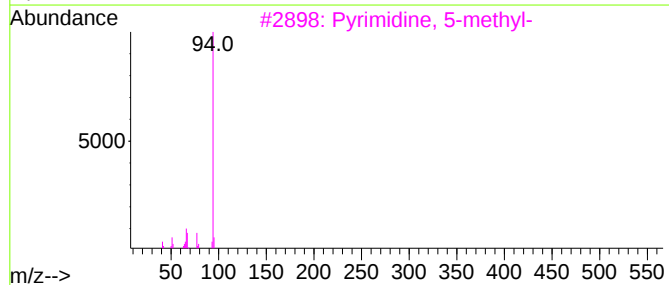
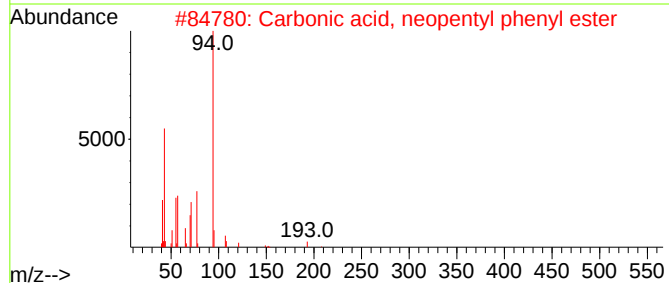
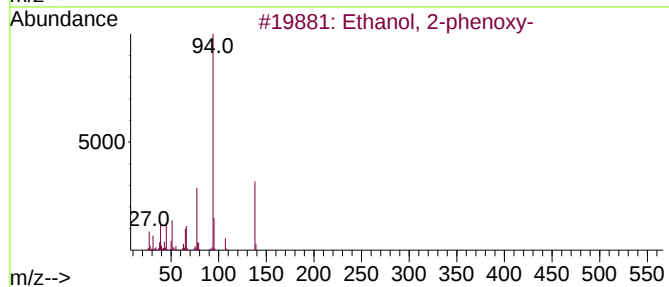
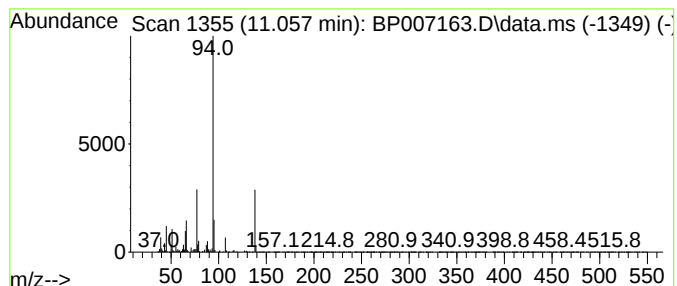
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Ethanol, 2-phenoxy- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.057	44.12 ng	4521060	Naphthalene-d8	10.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	95
2			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
3			Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	53
4			Benzene, ethoxy-	122	C8H10O	000103-73-1	50
5			Acetic acid, phenyl ester	136	C8H8O2	000122-79-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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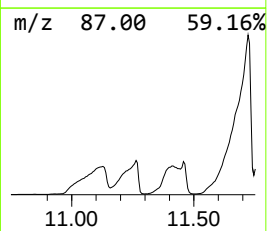
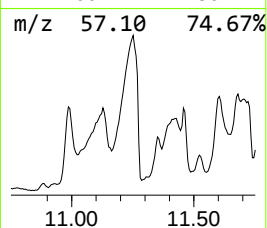
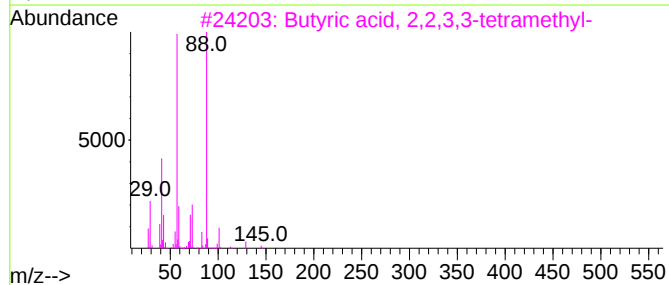
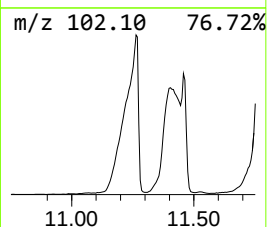
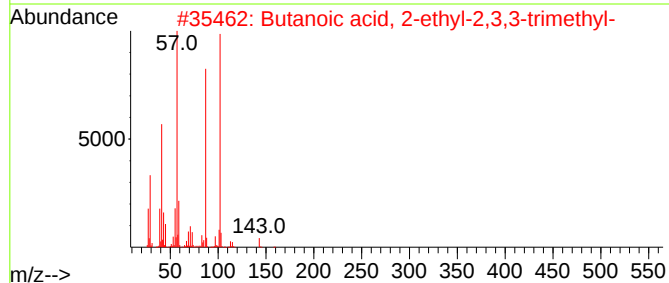
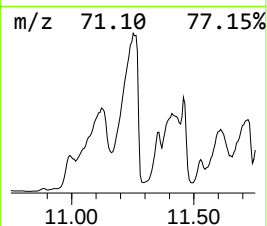
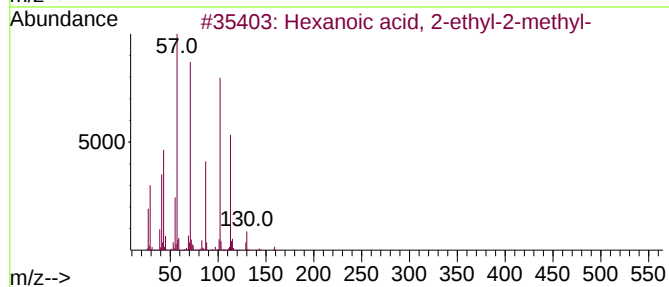
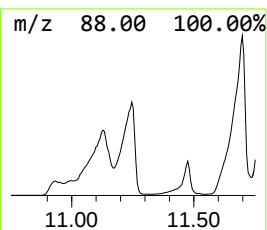
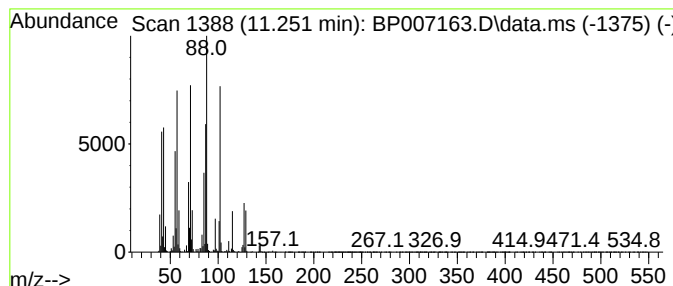
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown11.251 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.251	91.20 ng	9346480	Naphthalene-d8	10.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-2-methyl-	158	C9H18O2	001185-29-1	38
2			Butanoic acid, 2-ethyl-2,3,3-tri...	158	C9H18O2	038541-67-2	27
3			Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	22
4			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	22
5			Vinyl 2-ethyl-2,5-dimethylhexanoate	198	C12H22O2	1000498-24-9	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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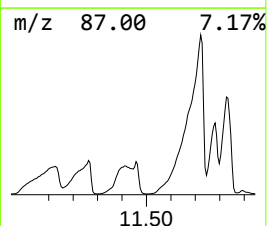
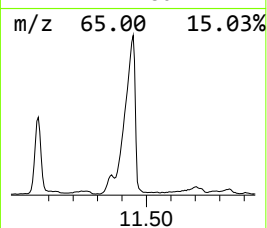
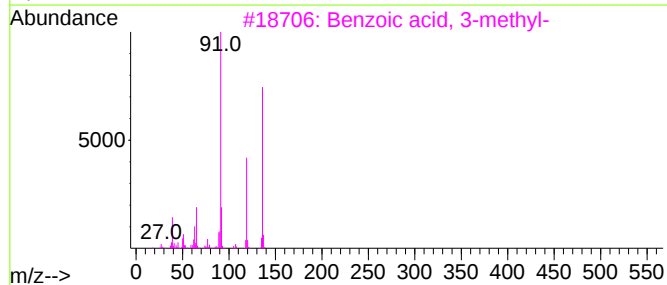
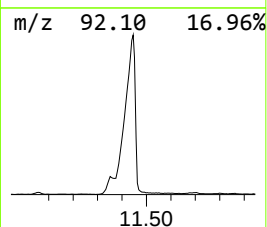
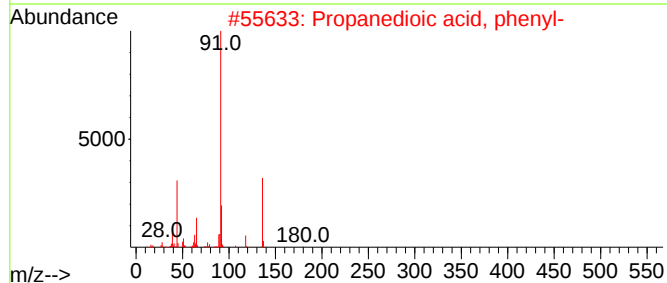
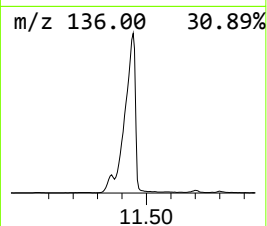
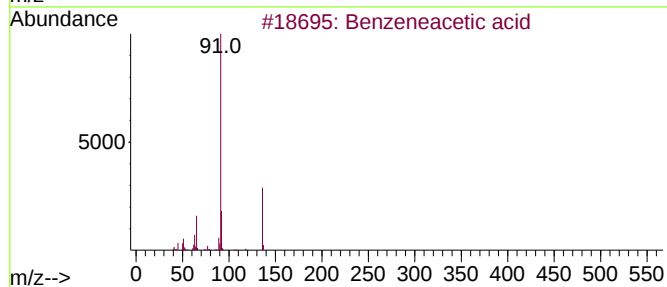
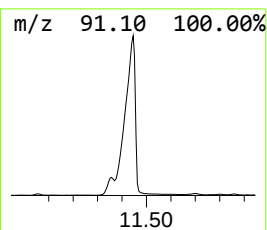
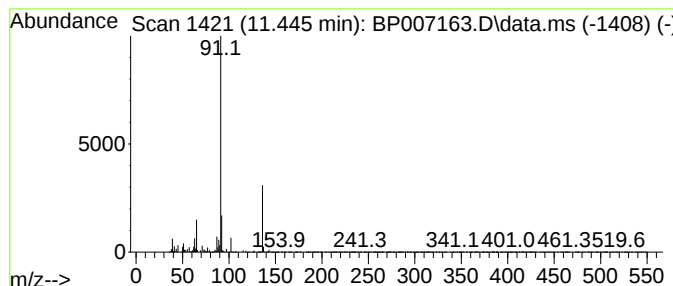
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Benzeneacetic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.445	126.71 ng	12985000	Naphthalene-d8	10.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	64
3			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	58
4			p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	53
5			Cyanamide, (phenylmethyl)-	132	C8H8N2	000622-77-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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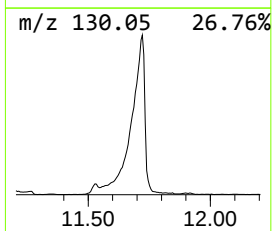
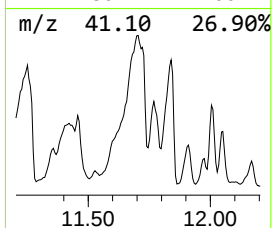
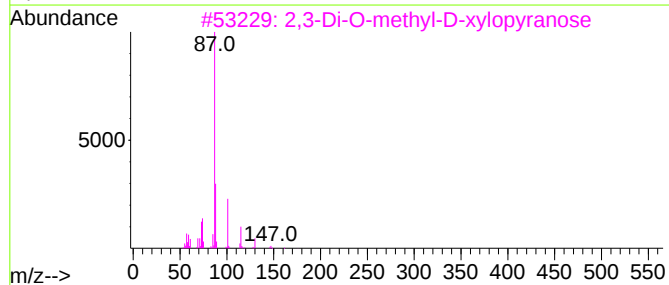
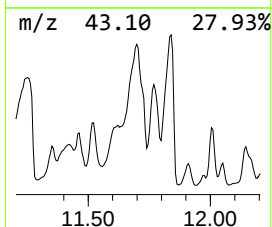
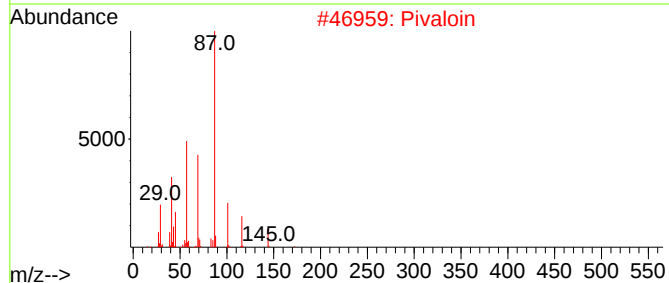
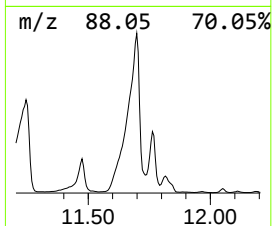
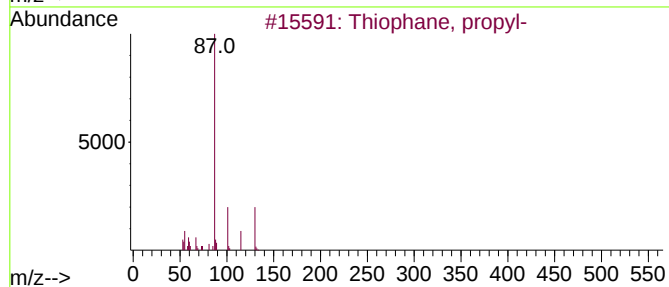
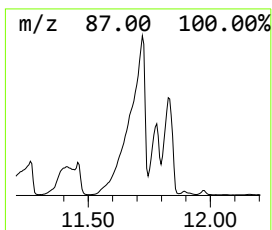
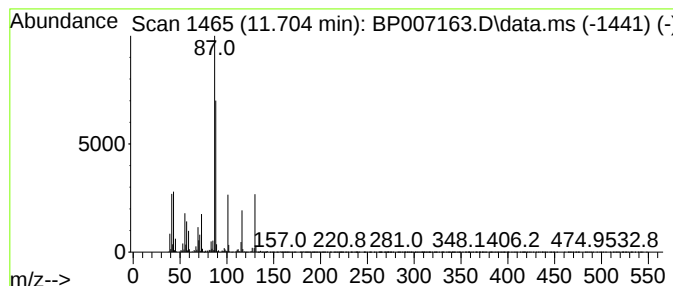
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Thiophane, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.704	177.01 ng	18140400	Naphthalene-d8	10.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	52
2			Pivaloin	172	C10H20O2	000815-66-7	47
3			2,3-Di-O-methyl-D-xylopyranose	178	C7H14O5	018186-26-0	42
4			Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	38
5			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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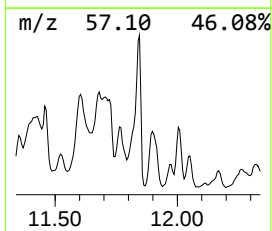
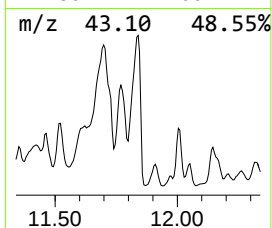
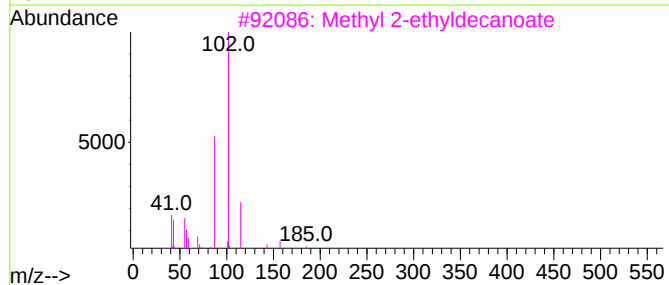
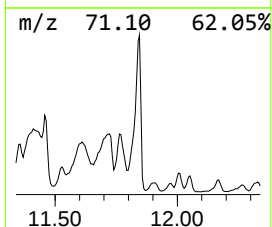
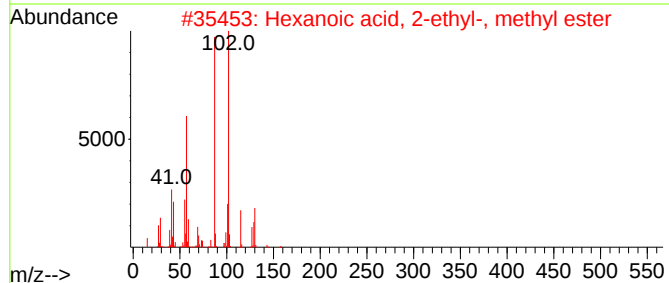
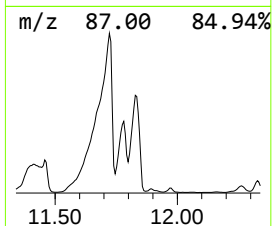
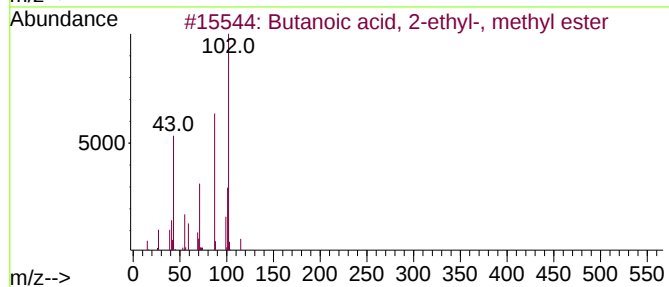
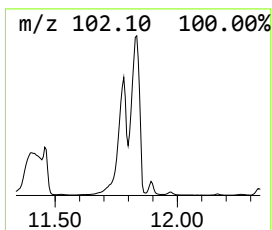
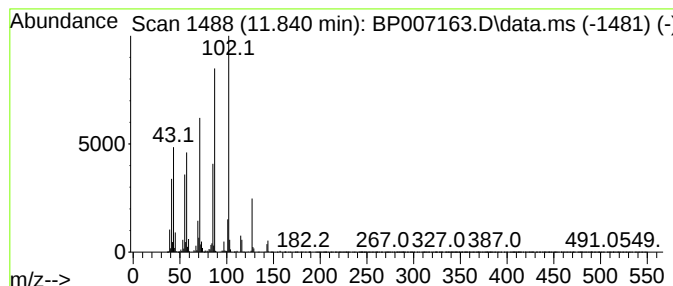
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown11.840 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.840	62.87 ng	6443080	Naphthalene-d8	10.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-ethyl-, methyl ...	130	C7H14O2	000816-11-5	42
2			Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	38
3			Methyl 2-ethyldecanoate	214	C13H26O2	020483-47-0	35
4			Pentanoic acid, 2-ethyl-, methyl...	144	C8H16O2	000816-16-0	25
5			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
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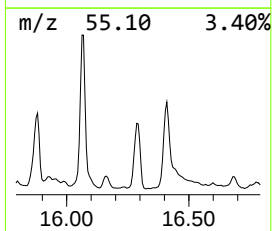
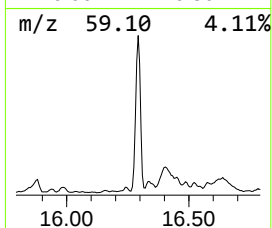
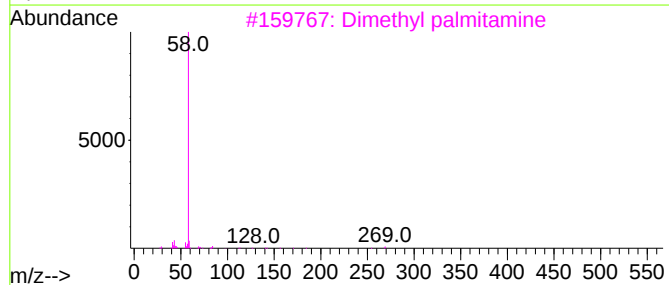
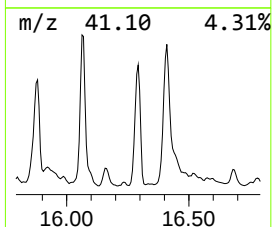
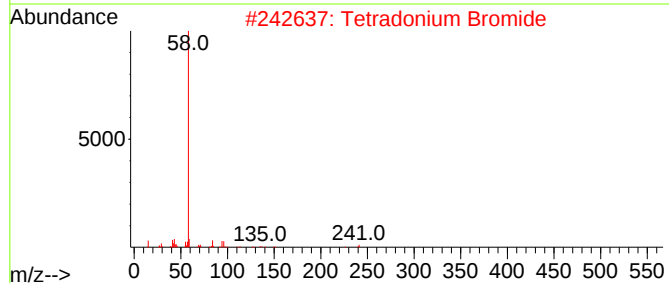
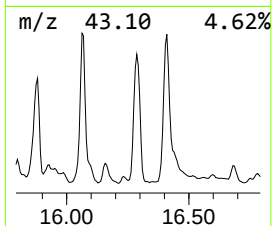
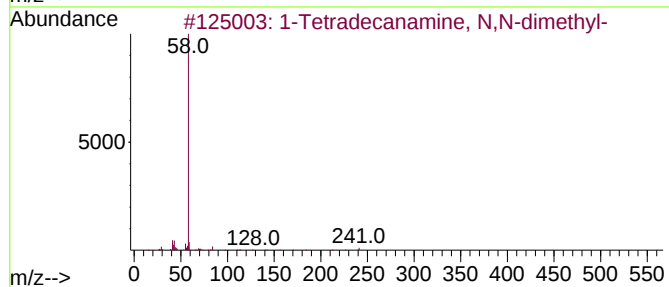
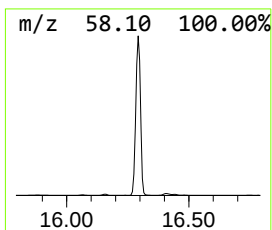
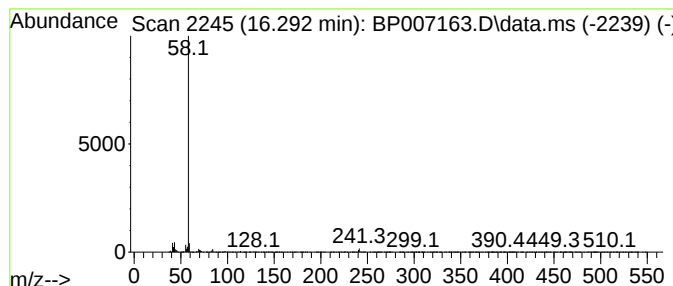
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 1-Tetradecanamine, N,N-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
16.292	76.45 ng	10568400	Phenanthrene-d10			17.269
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Tetradecanamine, N,N-dimethyl-		241	C16H35N	000112-75-4	90
2	Tetradonium Bromide		335	C17H38BrN	001119-97-7	78
3	Dimethyl palmitamine		269	C18H39N	000112-69-6	78
4	Dimantine		297	C20H43N	000124-28-7	72
5	1-Nonanamine, N,N-dimethyl-		171	C11H25N	017373-27-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

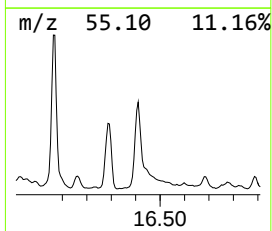
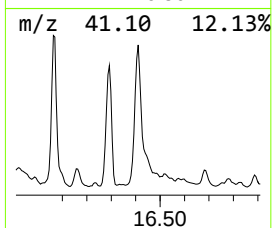
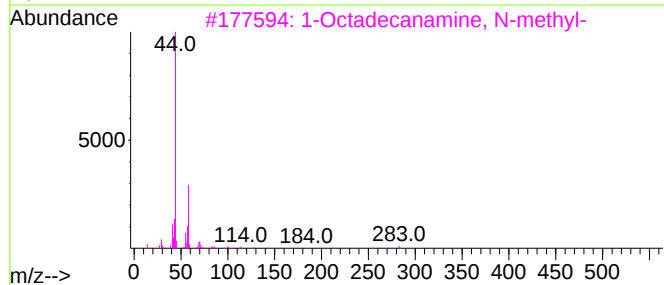
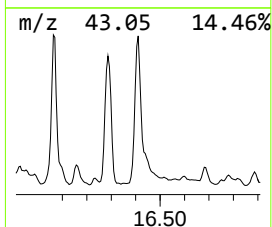
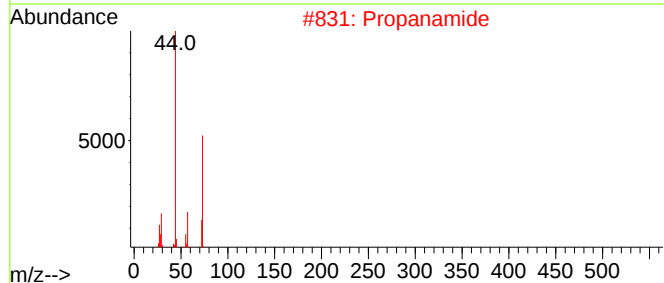
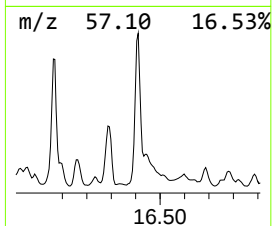
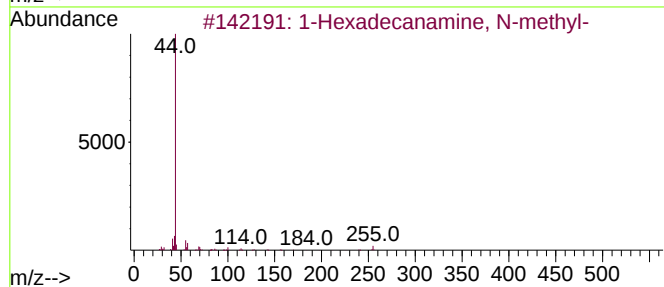
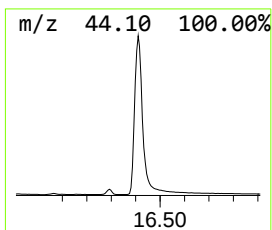
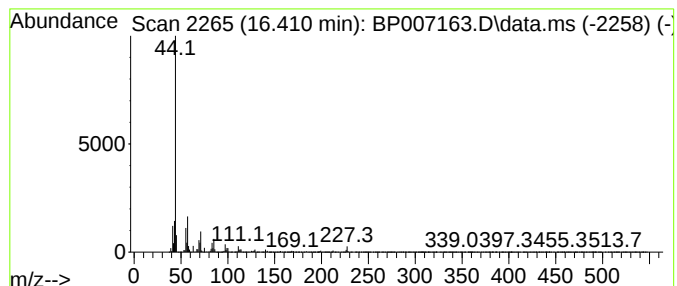
Instrument :
BNA_P
ClientSampleId :
20882

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 1-Hexadecanamine, N-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.410	90.41 ng	12499000	Phenanthrene-d10		17.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Hexadecanamine, N-methyl-		255	C17H37N	013417-08-8	53
2	Propanamide		73	C3H7NO	000079-05-0	53
3	1-Octadecanamine, N-methyl-		283	C19H41N	002439-55-6	45
4	2-Heptanamine, 5-methyl-		129	C8H19N	053907-81-6	42
5	Methylpent-4-enylamine		99	C6H13N	005831-72-1	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

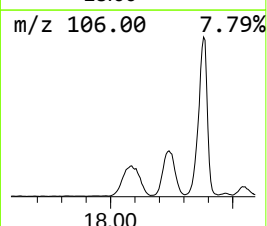
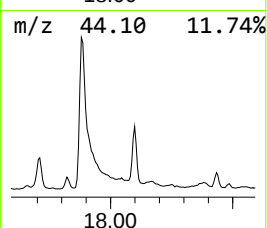
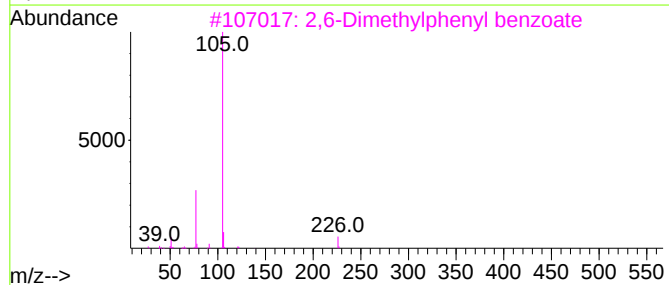
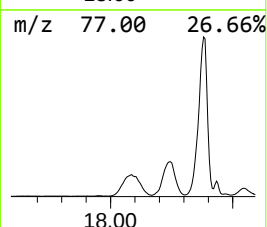
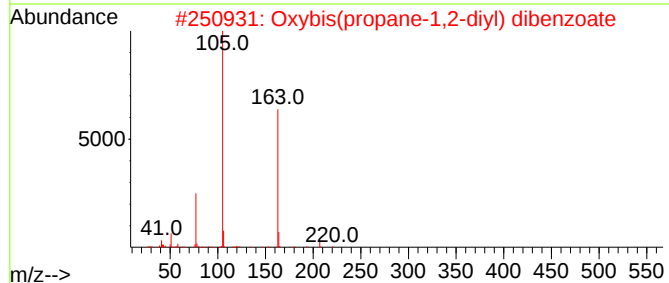
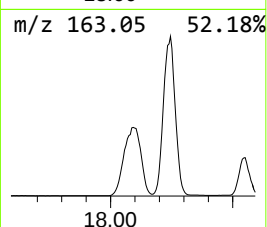
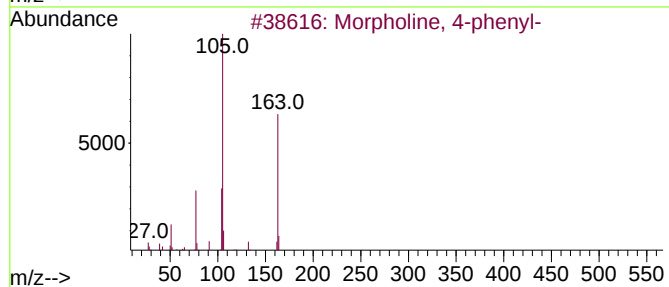
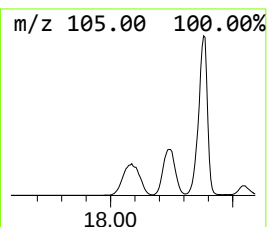
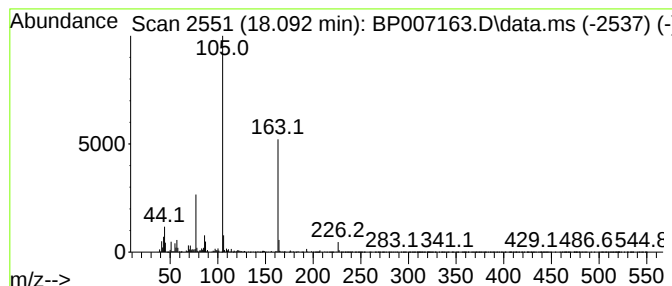
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Oxybis(propene-1,2-diyl) di... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.092	57.73 ng	7980680	Phenanthrene-d10	17.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
2	Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	59
3	2,6-Dimethylphenyl benzoate	226	C15H14O2	001871-36-9	42
4	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	35
5	Methyl undecyl phthalate	334	C20H30O4	070794-29-5	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

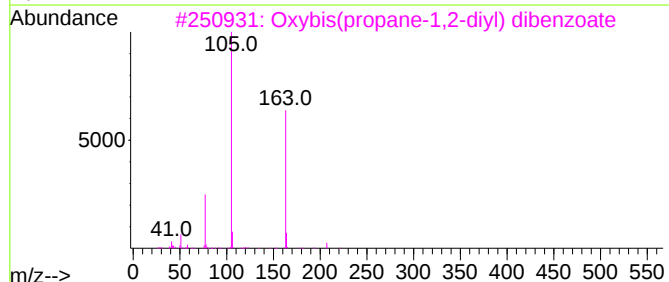
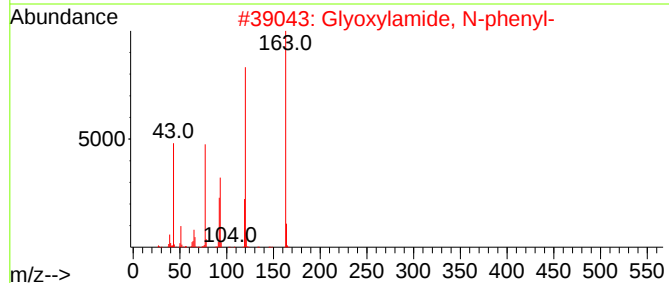
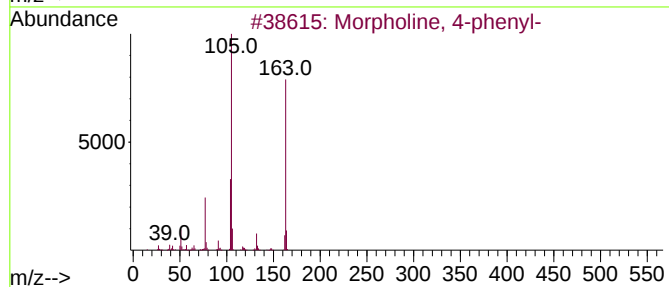
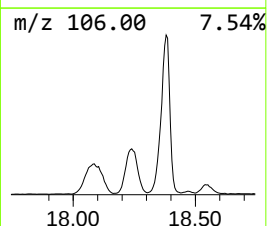
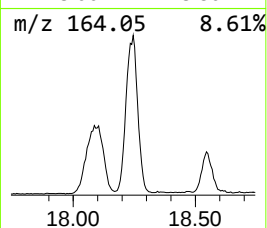
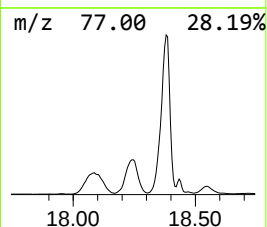
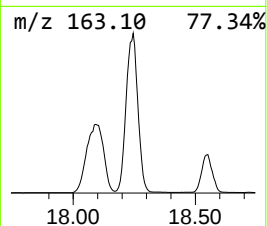
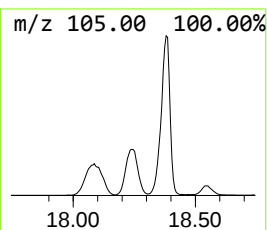
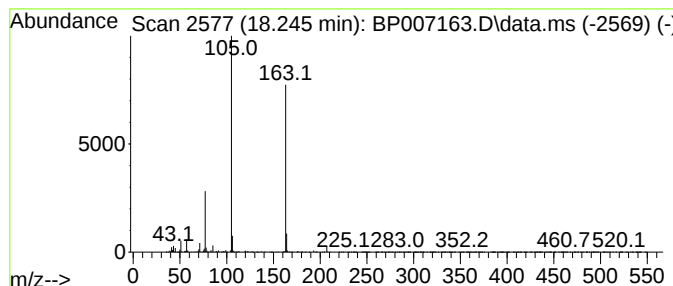
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Morpholine, 4-phenyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.245	64.45 ng	8909250	Phenanthrene-d10		17.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-		163	C10H13NO	000092-53-5	64
2	Glyoxylamide, N-phenyl-		163	C9H9NO2	032331-52-5	53
3	Oxybis(propane-1,2-diyl) dibenzoate		342	C20H22O5	000094-03-1	49
4	Phenylglyoxylic acid, neopentyl ...		220	C13H16O3	1000453-45-9	22
5	Phenylglyoxylic acid, 2-methylbu...		220	C13H16O3	1010453-46-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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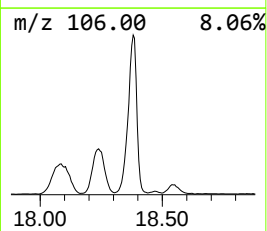
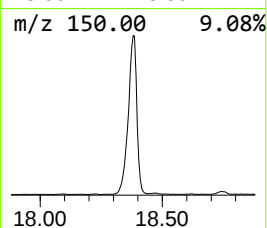
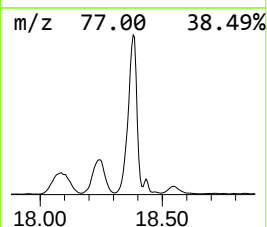
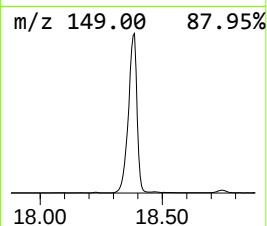
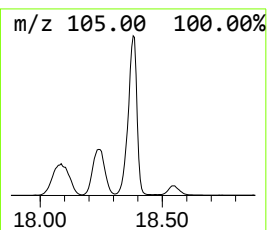
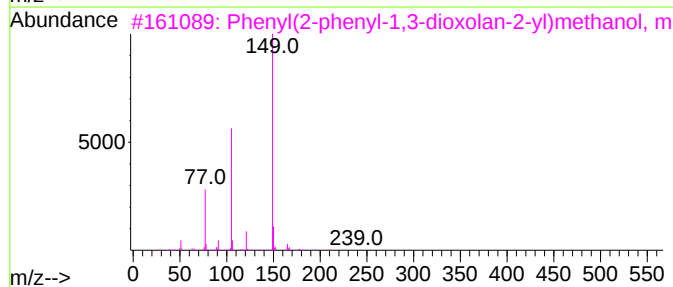
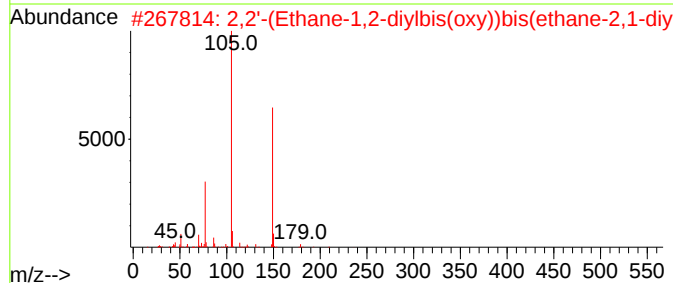
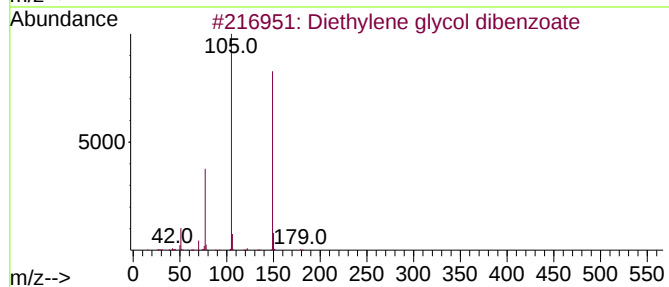
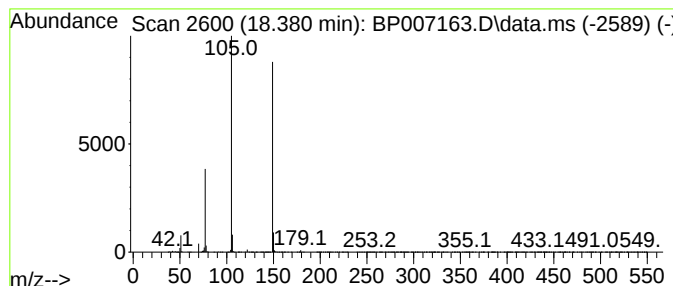
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.380	155.44 ng	21488600	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
3			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
4			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
5			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007163.D
Acq On : 24 Sep 2021 17:41
Operator : CG/JU
Sample : M3875-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one,...	3.787	73.9	ng	5587690	1	7.887	1512200	20.0
Butanoic acid	4.169	52.5	ng	3972040	1	7.887	1512200	20.0
1,3-Dioxolane, ...	4.216	57.1	ng	4320080	1	7.887	1512200	20.0
3-Hexen-2-one	4.405	254.1	ng	19209700	1	7.887	1512200	20.0
1,4-Dioxane, 2,...	4.516	60.2	ng	4554380	1	7.887	1512200	20.0
Propanedioic acid	4.893	77.8	ng	5886320	1	7.887	1512200	20.0
2-Pentanone, 4-...	5.005	65.7	ng	4965650	1	7.887	1512200	20.0
Pentanoic acid,...	6.622	96.7	ng	7310530	1	7.887	1512200	20.0
unknown8.934	8.934	43.1	ng	3258880	1	7.887	1512200	20.0
Levogluconenone	9.410	93.7	ng	9606730	2	10.687	2049650	20.0
Ethanol, 2-phen...	11.057	44.1	ng	4521060	2	10.687	2049650	20.0
unknown11.251	11.251	91.2	ng	9346480	2	10.687	2049650	20.0
Benzeneacetic acid	11.445	126.7	ng	12985000	2	10.687	2049650	20.0
Thiophane, propyl-	11.704	177.0	ng	18140400	2	10.687	2049650	20.0
unknown11.840	11.840	62.9	ng	6443080	2	10.687	2049650	20.0
1-Tetradecanami...	16.292	76.5	ng	10568400	4	17.269	2764900	20.0
1-Hexadecanamin...	16.410	90.4	ng	12499000	4	17.269	2764900	20.0
Oxybis(propane-...	18.092	57.7	ng	7980680	4	17.269	2764900	20.0
Morpholine, 4-p...	18.245	64.5	ng	8909250	4	17.269	2764900	20.0
Diethylene glyc...	18.380	155.4	ng	21488600	4	17.269	2764900	20.0