

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
 Data File : BM029524.D
 Acq On : 16 Apr 2021 16:31
 Operator : CG/JU
 Sample : M1998-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-3A

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_M\Methods\8270-BM040121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029524.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.922	3	6	17	rVB	953178	1119974	29.59%	3.153%
2	4.816	323	328	338	rBV	211030	301120	7.96%	0.848%
3	5.269	399	405	413	rBV	1353423	1915518	50.61%	5.392%
4	6.852	664	674	690	rBV2	1464724	3121640	82.48%	8.788%
5	7.310	746	752	758	rBV	70650	121369	3.21%	0.342%
6	7.463	772	778	791	rBV	83044	151749	4.01%	0.427%
7	7.669	804	813	821	rVV	381081	630340	16.65%	1.774%
8	7.740	821	825	831	rVB	68981	106901	2.82%	0.301%
9	8.216	899	906	912	rBV3	35147	73979	1.95%	0.208%
10	8.440	937	944	949	rBV9	21345	46746	1.24%	0.132%
11	8.769	990	1000	1003	rBV9	26582	72751	1.92%	0.205%
12	8.822	1003	1009	1016	rVV	880391	1429065	37.76%	4.023%
13	8.987	1032	1037	1040	rBV4	28139	54174	1.43%	0.153%
14	9.251	1069	1082	1087	rBV5	35300	97487	2.58%	0.274%
15	9.381	1097	1104	1109	rVB5	37276	82685	2.18%	0.233%
16	9.640	1143	1148	1156	rBV6	40429	71074	1.88%	0.200%
17	9.893	1183	1191	1199	rBV7	26605	86184	2.28%	0.243%
18	10.198	1238	1243	1260	rVB2	88172	237028	6.26%	0.667%
19	10.451	1277	1286	1292	rBV	501000	878657	23.22%	2.473%
20	10.622	1311	1315	1321	rBV	88442	130069	3.44%	0.366%
21	10.945	1366	1370	1376	rVB2	39706	65706	1.74%	0.185%
22	11.140	1395	1403	1404	rBV8	31994	66016	1.74%	0.186%
23	11.298	1424	1430	1436	rVV7	34321	78183	2.07%	0.220%
24	11.381	1438	1444	1450	rVB5	43157	101448	2.68%	0.286%
25	11.487	1457	1462	1471	rBV	151941	315511	8.34%	0.888%
26	11.645	1484	1489	1492	rBV6	23622	38475	1.02%	0.108%
27	11.745	1502	1506	1510	rVB3	44345	60335	1.59%	0.170%
28	11.892	1526	1531	1536	rBV2	66163	110716	2.93%	0.312%
29	11.951	1536	1541	1550	rVB	117365	222267	5.87%	0.626%
30	12.116	1558	1569	1576	rVB6	70786	233115	6.16%	0.656%
31	12.222	1578	1587	1590	rBV4	62479	149609	3.95%	0.421%
32	12.340	1603	1607	1610	rBV6	25719	46235	1.22%	0.130%
33	12.387	1611	1615	1624	rVB2	40528	90538	2.39%	0.255%
34	12.528	1637	1639	1643	rVB2	44786	54584	1.44%	0.154%
35	12.587	1644	1649	1655	rVB4	33689	74524	1.97%	0.210%
36	12.716	1667	1671	1673	rBV2	39937	61845	1.63%	0.174%

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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_M\Methods\8270-BM040121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.804	1682	1686	1690	rBV3	50178	91945	2.43%	0.259%
38	12.851	1690	1694	1699	rVV	212284	311909	8.24%	0.878%
39	12.928	1700	1707	1714	rVB	1872828	2837392	74.97%	7.987%
40	13.092	1732	1735	1737	rBV2	41636	53209	1.41%	0.150%
41	13.234	1756	1759	1764	rVB6	51220	73897	1.95%	0.208%
42	13.634	1823	1827	1831	rBV2	44337	84096	2.22%	0.237%
43	13.734	1839	1844	1848	rBV3	173329	261692	6.91%	0.737%
44	13.804	1848	1856	1860	rVV3	331315	576880	15.24%	1.624%
45	13.851	1860	1864	1870	rVV4	107381	189628	5.01%	0.534%
46	13.922	1874	1876	1880	rVB2	45338	55257	1.46%	0.156%
47	14.022	1889	1893	1895	rBV3	50290	78182	2.07%	0.220%
48	14.145	1910	1914	1922	rVB4	155430	293941	7.77%	0.827%
49	14.222	1923	1927	1932	rBV3	98078	147068	3.89%	0.414%
50	14.310	1934	1942	1950	rVB	714871	1201651	31.75%	3.383%
51	14.845	2029	2033	2040	rBV3	182589	345656	9.13%	0.973%
52	15.175	2087	2089	2094	rBV2	56119	66951	1.77%	0.188%
53	15.586	2153	2159	2163	rBV	354246	570187	15.07%	1.605%
54	15.733	2181	2184	2189	rBV7	84029	161153	4.26%	0.454%
55	15.798	2190	2195	2202	rVB2	696162	1048521	27.70%	2.952%
56	16.063	2232	2240	2251	rBV	768619	1419478	37.51%	3.996%
57	16.151	2252	2255	2262	rBV4	76932	163295	4.31%	0.460%
58	16.880	2375	2379	2390	rVB	423784	711133	18.79%	2.002%
59	17.057	2404	2409	2413	rBV	752151	1151294	30.42%	3.241%
60	17.157	2423	2426	2430	rBV	156826	202423	5.35%	0.570%
61	17.963	2560	2563	2568	rVB2	123322	222053	5.87%	0.625%
62	18.257	2611	2613	2622	rVB3	110086	155093	4.10%	0.437%
63	18.986	2733	2737	2743	rBV	290925	392712	10.38%	1.106%
64	19.116	2755	2759	2764	rVB	261565	325240	8.59%	0.916%
65	19.474	2817	2820	2830	rVB2	315932	606141	16.02%	1.706%
66	19.686	2851	2856	2868	rVB	3014768	3784708	100.00%	10.654%
67	19.974	2902	2905	2908	rVB2	128106	141569	3.74%	0.399%
68	20.957	3069	3072	3083	rVB	855704	1058629	27.97%	2.980%
69	21.162	3103	3107	3113	rVB	948587	1089213	28.78%	3.066%
70	21.233	3114	3119	3123	rBV2	1065469	1437888	37.99%	4.048%
71	23.445	3490	3495	3502	rVB2	668137	1201749	31.75%	3.383%
72	24.445	3661	3665	3671	rBV2	270490	513699	13.57%	1.446%

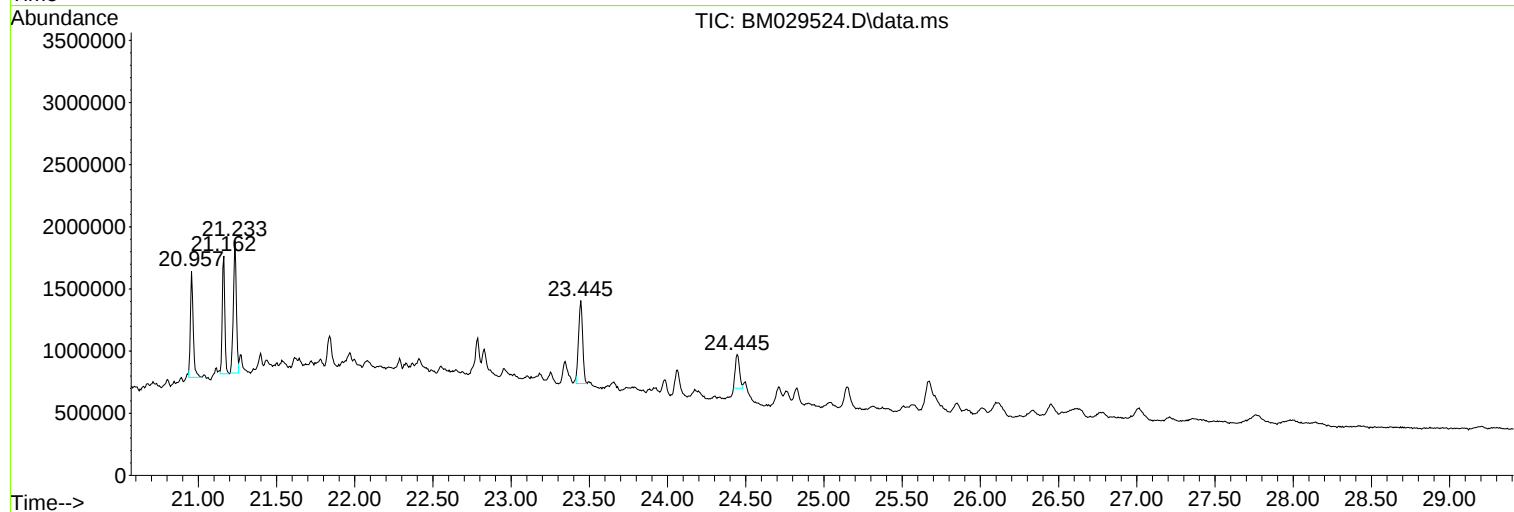
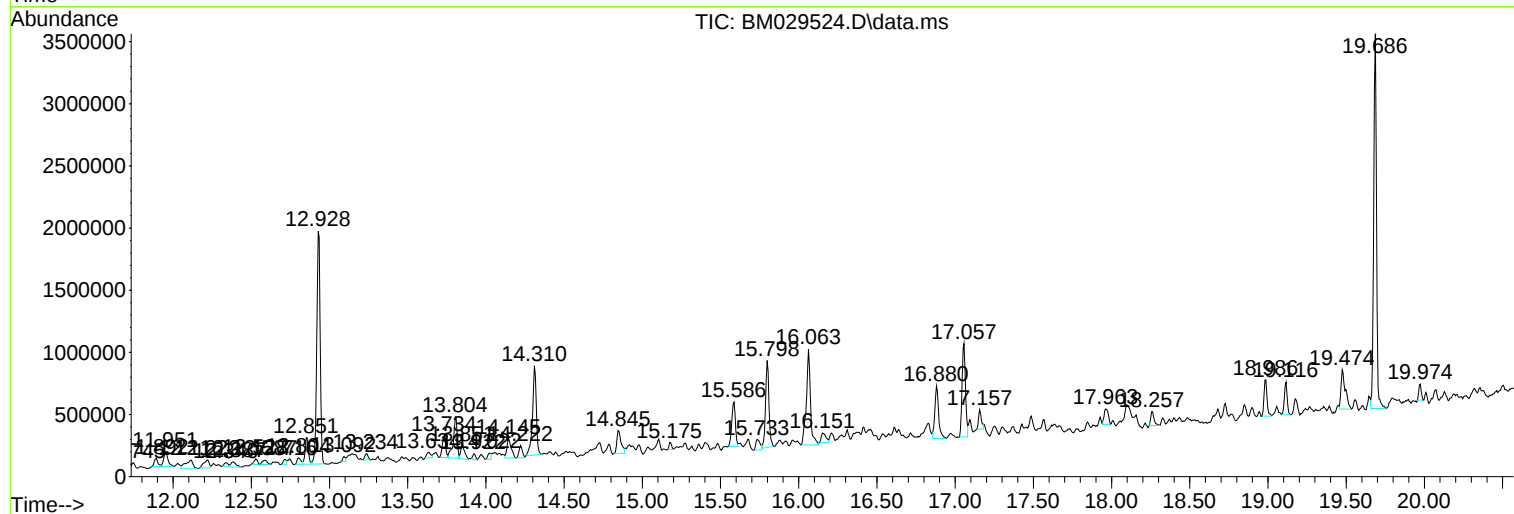
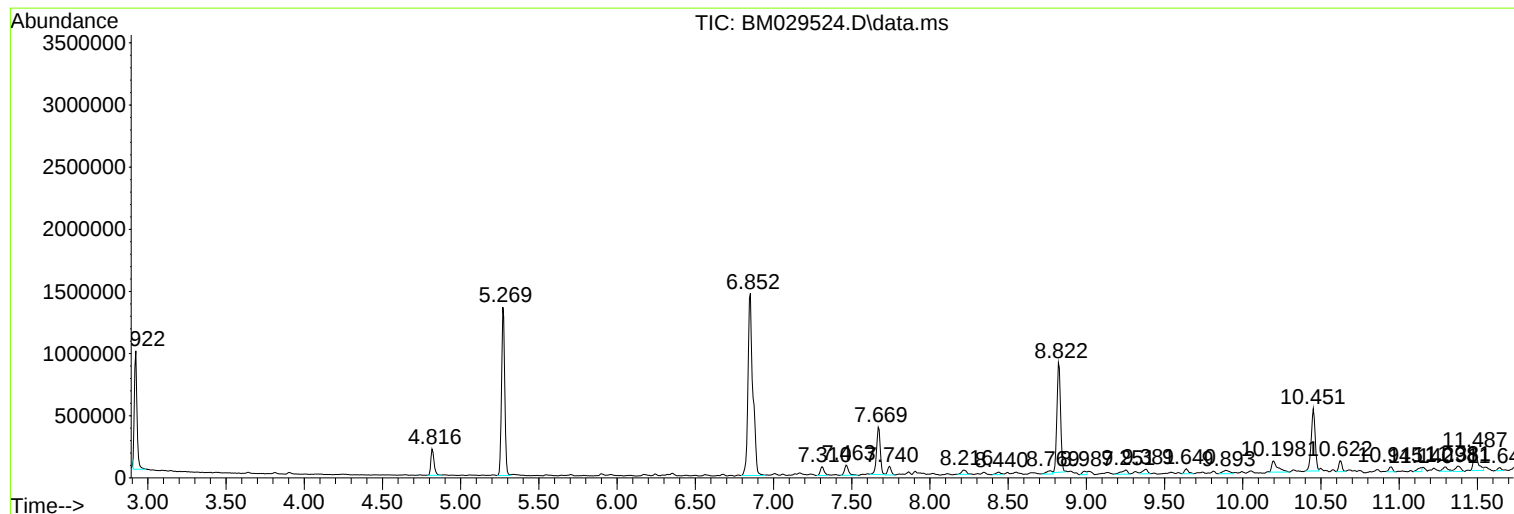
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Instrument :
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ClientSampleId :
SB-3A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
Operator : CG/JU
Sample : M1998-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-3A

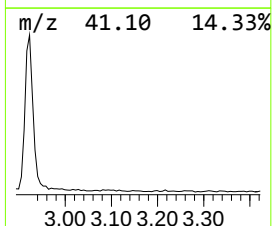
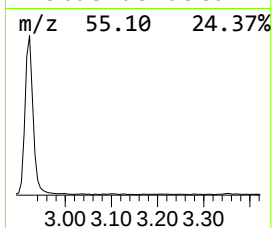
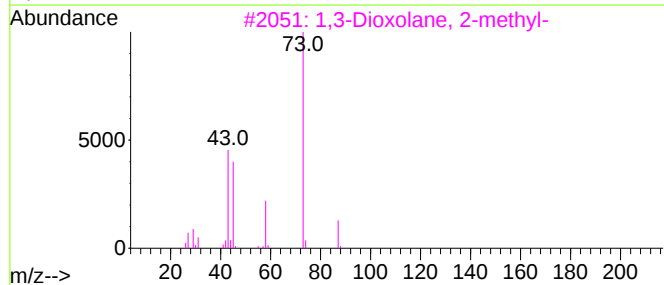
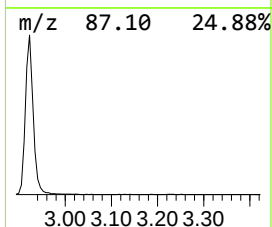
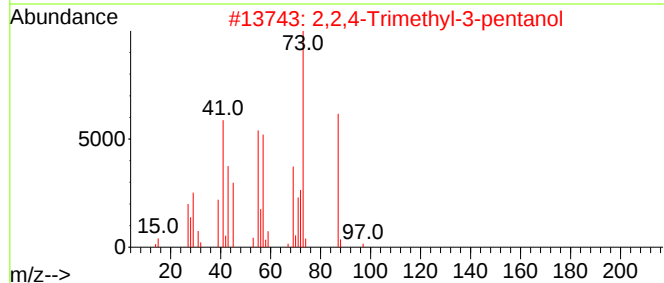
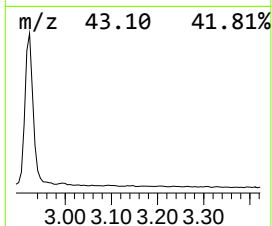
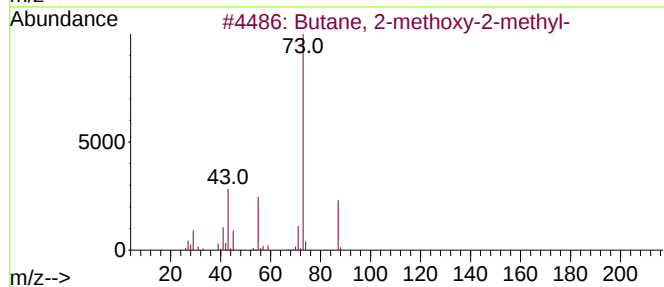
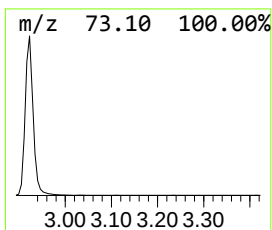
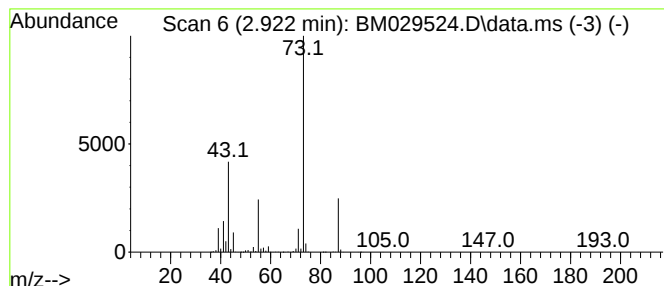
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.922	35.54 ng	1119970	1,4-Dichlorobenzene-d4	7.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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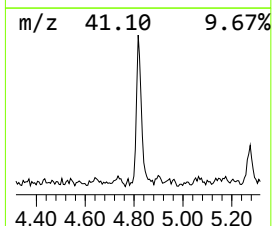
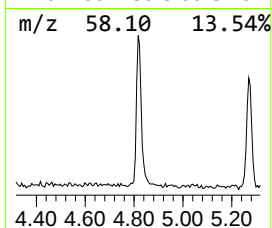
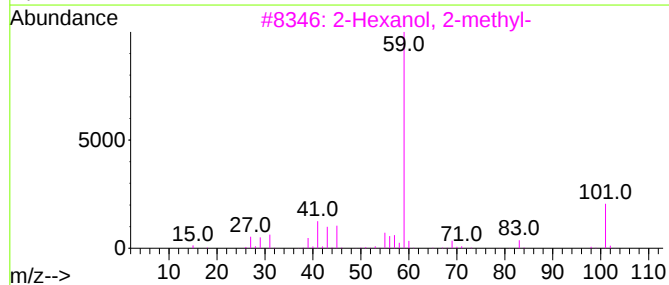
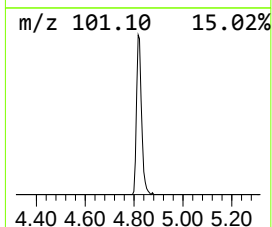
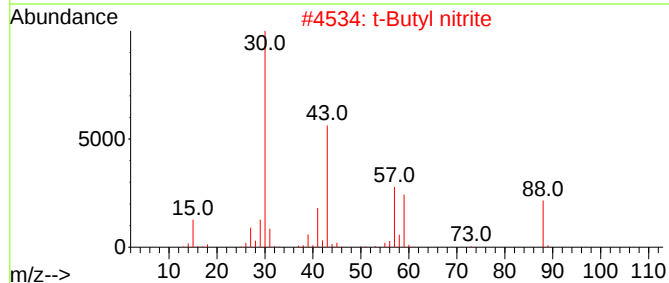
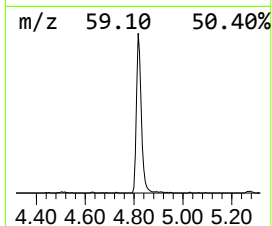
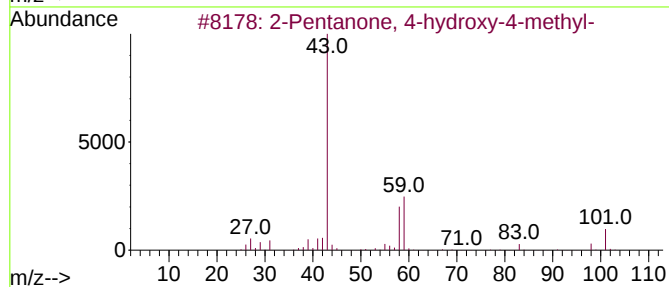
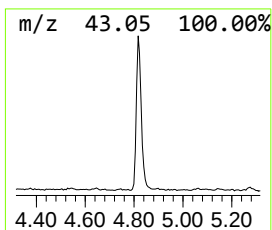
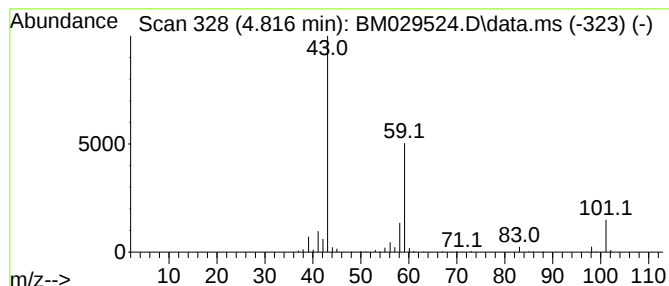
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.816	9.55 ng	301120	1,4-Dichlorobenzene-d4	7.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		t-Butyl nitrite	103	C4H9NO2	000540-80-7	50
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Guanidine	59	CH5N3	000113-00-8	9



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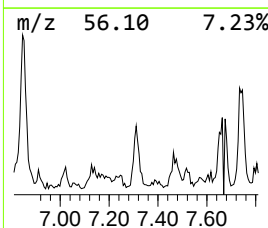
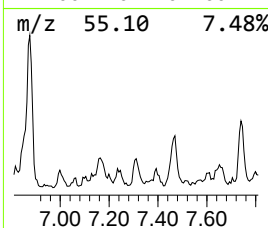
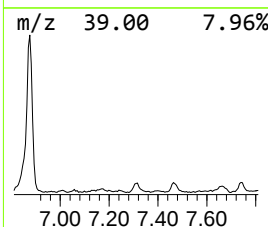
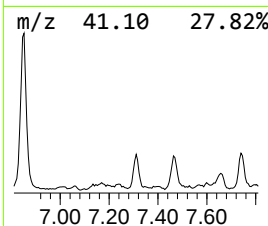
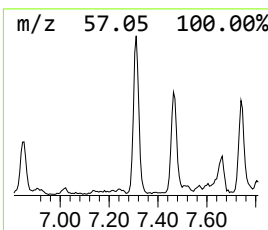
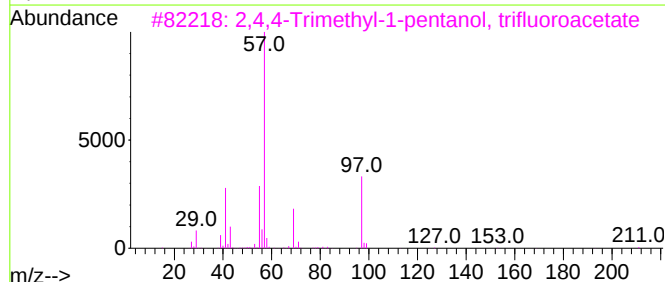
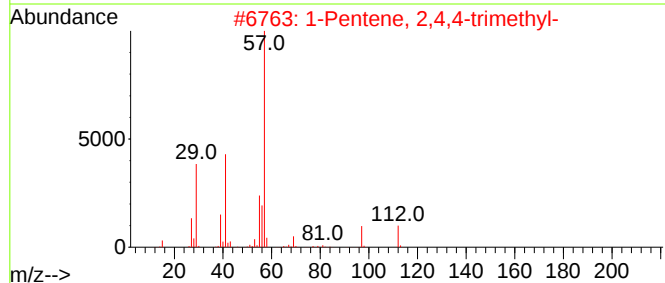
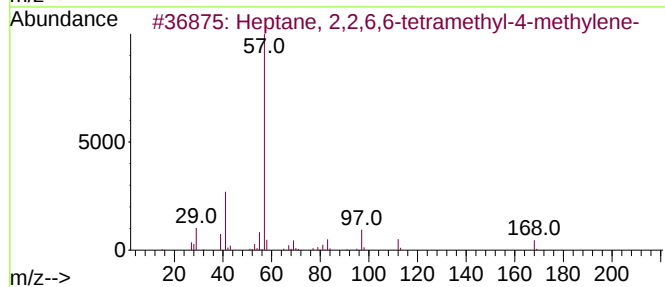
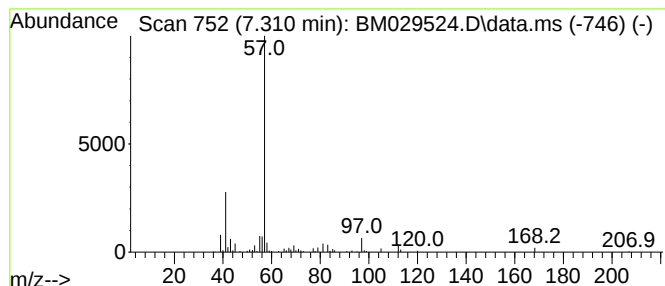
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptane, 2,2,6,6-tetramethyl... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.310	3.85 ng	121369	1,4-Dichlorobenzene-d4	7.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,2,6,6-tetramethyl-4-m...	168	C12H24	000141-70-8	59
2			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	47
3			2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	43
4			Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	42
5			Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	40



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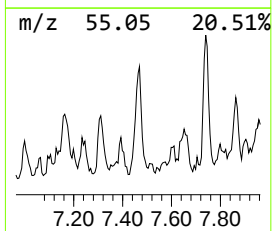
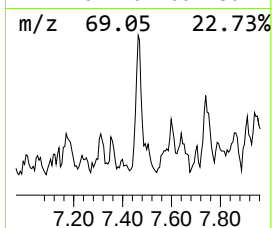
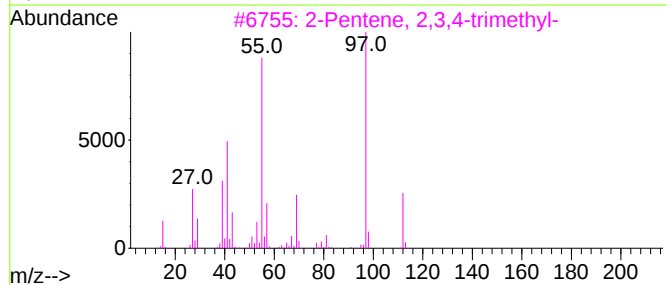
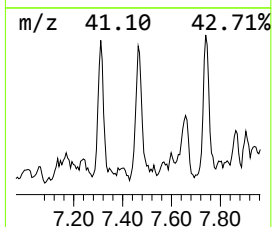
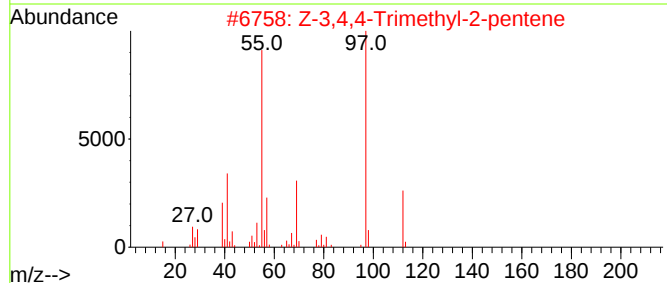
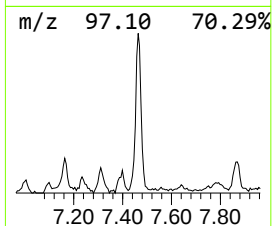
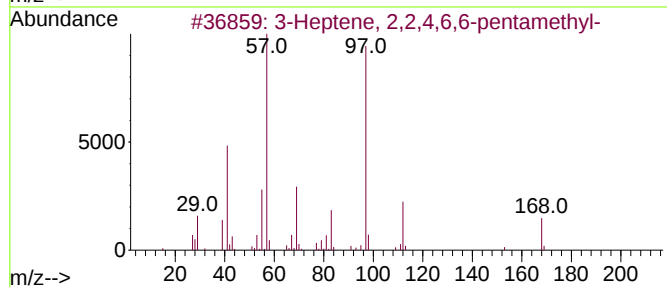
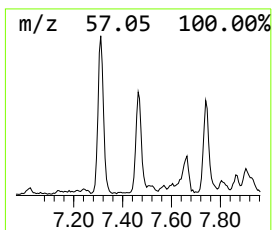
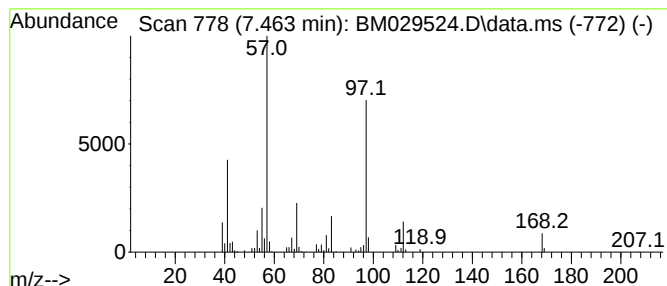
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Heptene, 2,2,4,6,6-pentam... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.463	4.81 ng	151749	1,4-Dichlorobenzene-d4	7.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptene, 2,2,4,6,6-pentamethyl-	168	C12H24	000123-48-8	83
2			Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	58
3			2-Pentene, 2,3,4-trimethyl-	112	C8H16	000565-77-5	50
4			Heptane, 2,2,6,6-tetramethyl-4-m...	168	C12H24	000141-70-8	50
5			2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
Operator : CG/JU
Sample : M1998-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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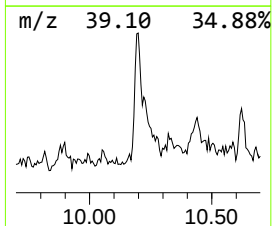
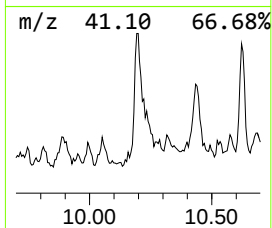
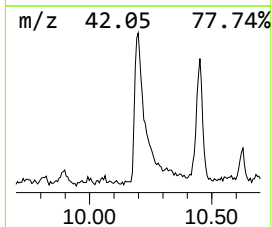
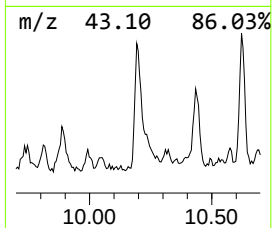
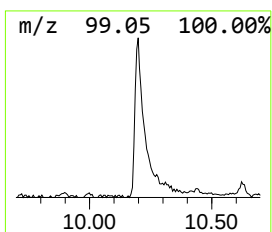
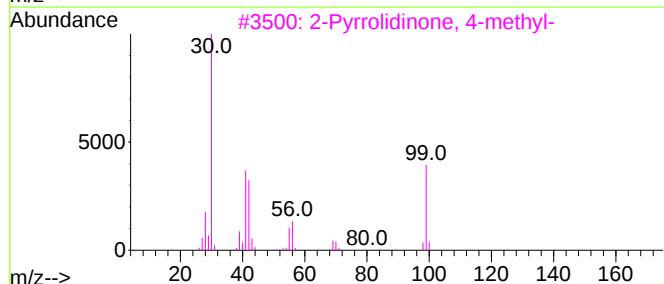
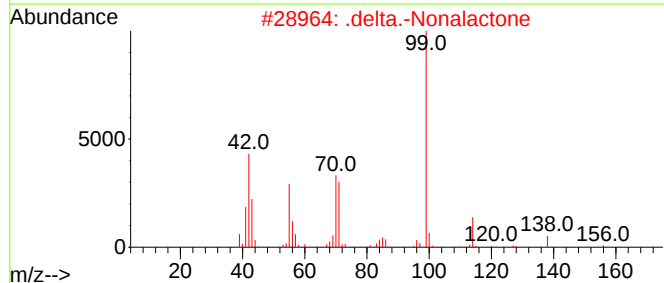
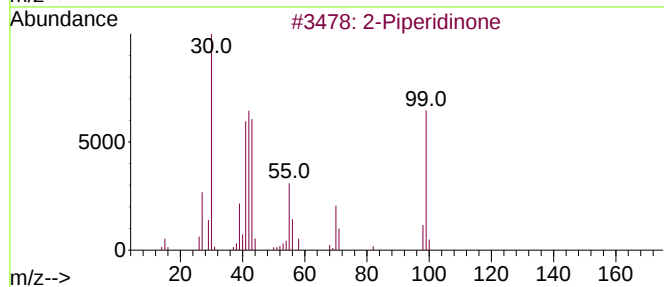
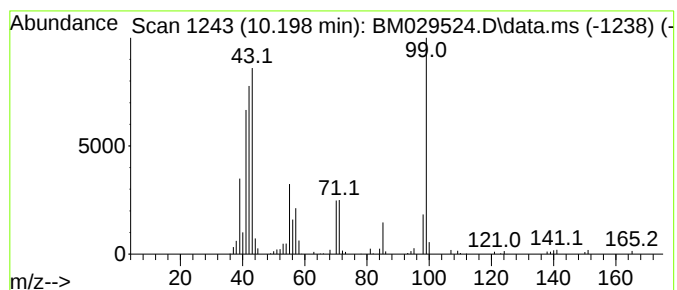
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Piperidinone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.198	5.40 ng	237028	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Piperidinone	99	C5H9NO	000675-20-7	90
2			.delta.-Nonalactone	156	C9H16O2	003301-94-8	72
3			2-Pyrrolidinone, 4-methyl-	99	C5H9NO	1000197-00-3	53
4			4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	46
5			2-Ethylbutyric acid, isohexyl ester	200	C12H24O2	1000340-24-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
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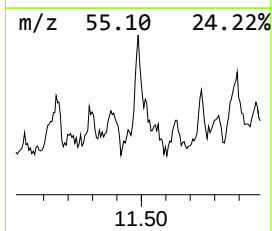
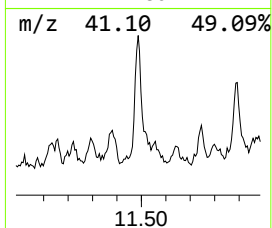
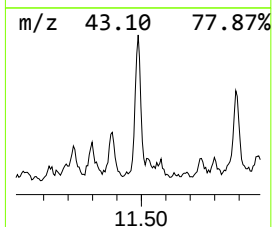
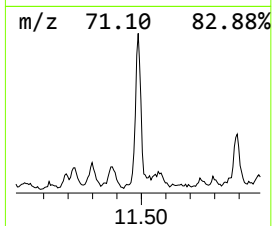
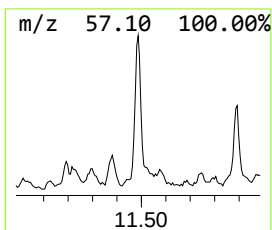
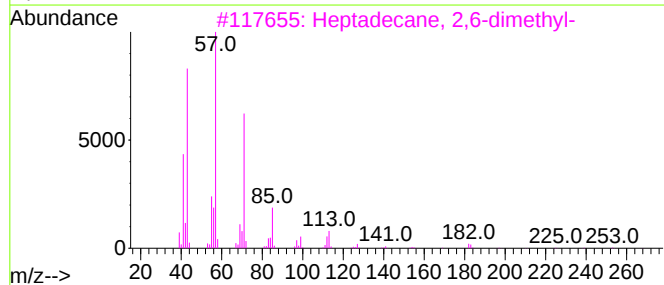
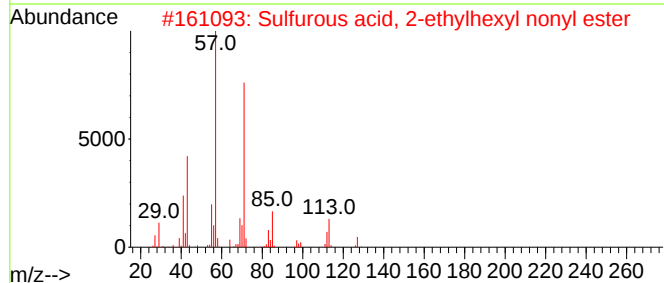
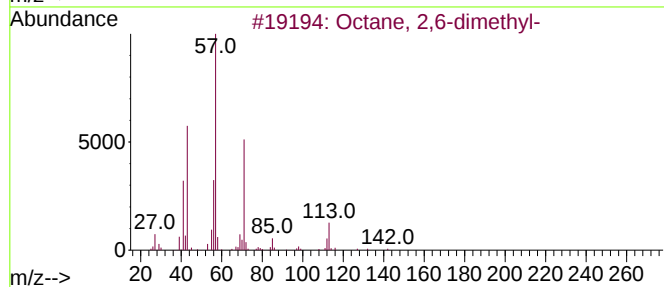
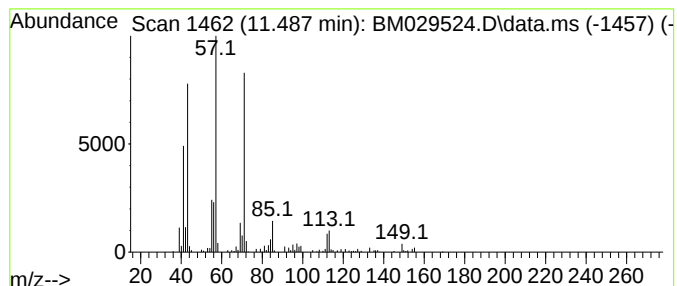
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octane, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.487	7.18 ng	315511	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	86
2			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	72
3			Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	72
4			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
5			Eicosane	282	C20H42	000112-95-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
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Misc :
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ClientSampleId :
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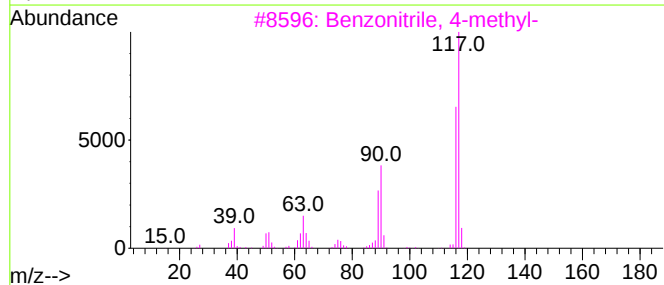
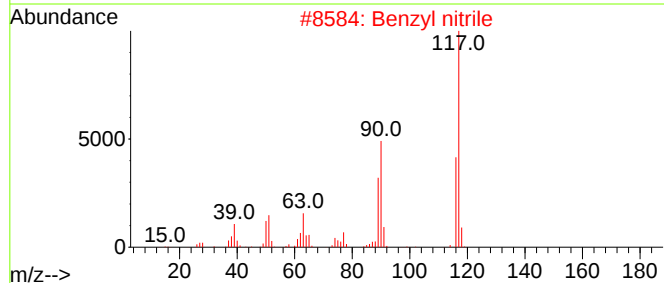
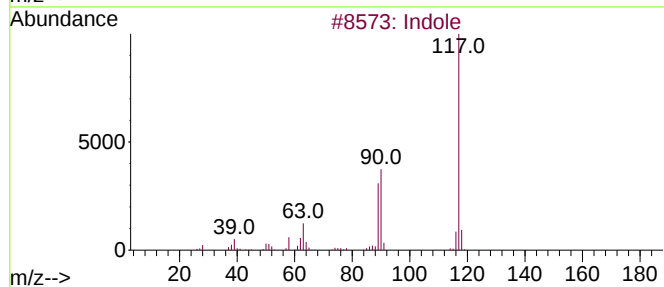
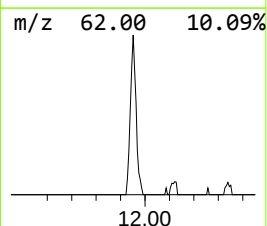
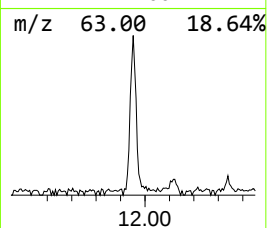
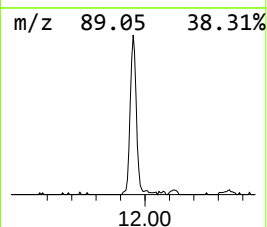
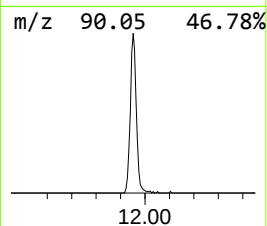
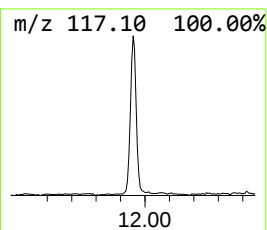
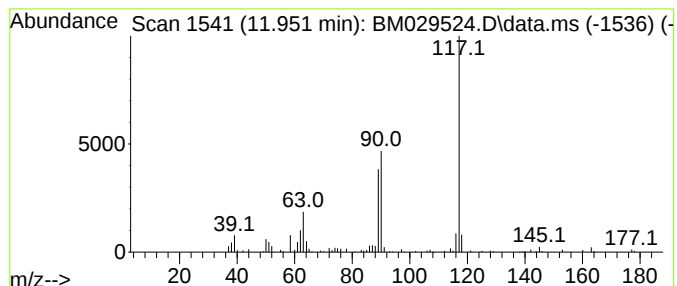
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Indole Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	5.06 ng	222267	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	94
2			Benzyl nitrile	117	C8H7N	000140-29-4	91
3			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	91
4			Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	91
5			Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
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Misc :
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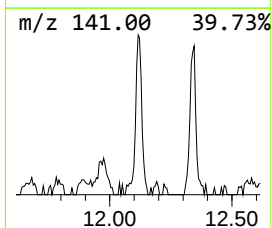
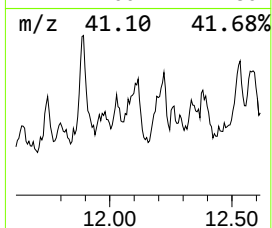
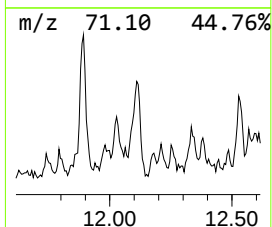
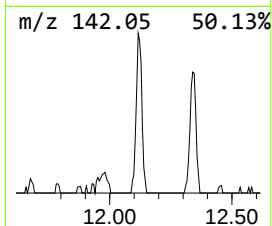
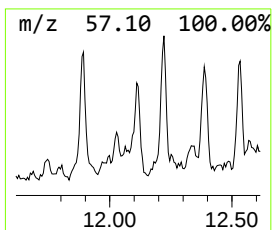
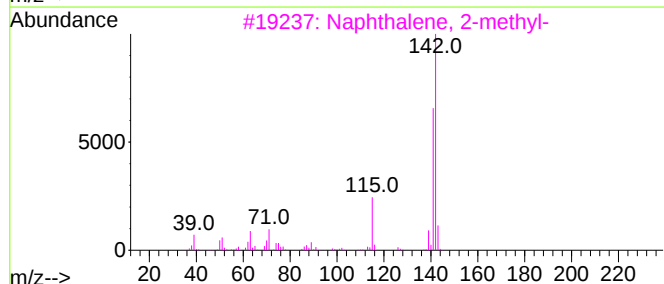
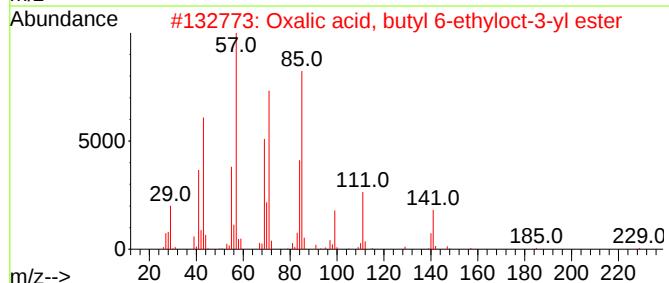
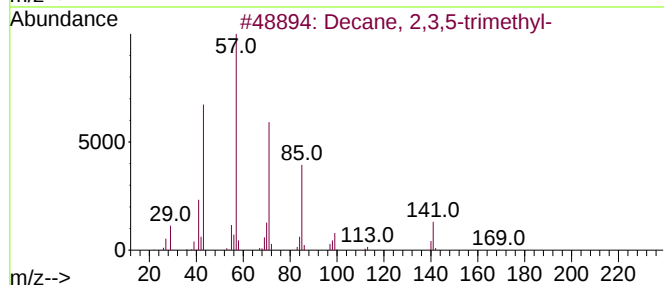
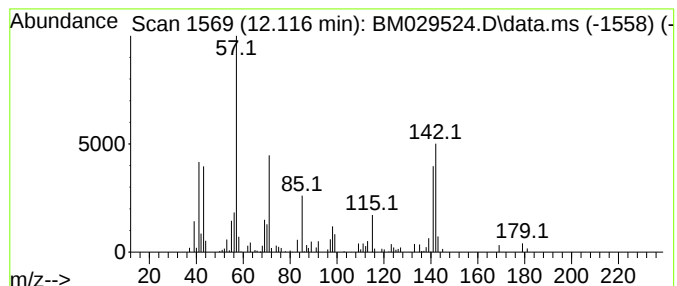
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Decane, 2,3,5-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.116	5.31 ng	233115	Naphthalene-d8	10.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	50
2			Oxalic acid, butyl 6-ethyloct-3-...	286	C16H30O4	1000309-34-2	50
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	43
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	38
5			Undecane, 5-ethyl-	184	C13H28	017453-94-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
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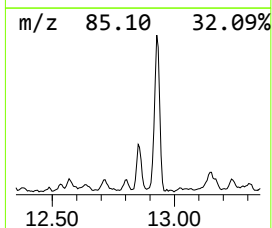
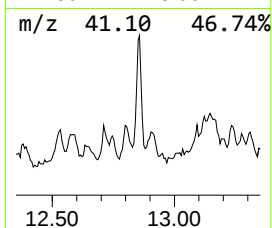
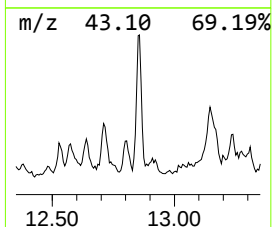
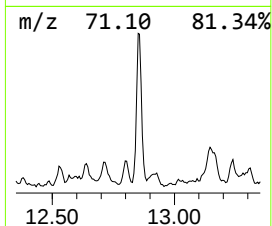
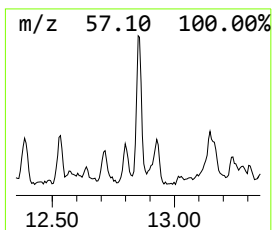
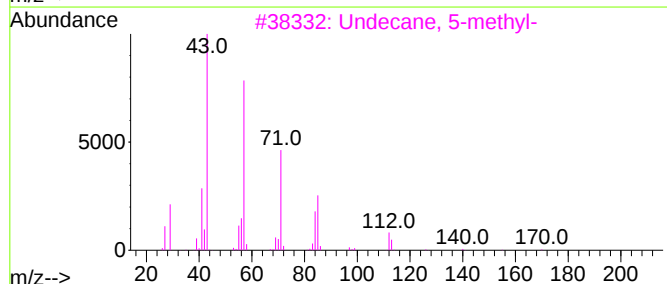
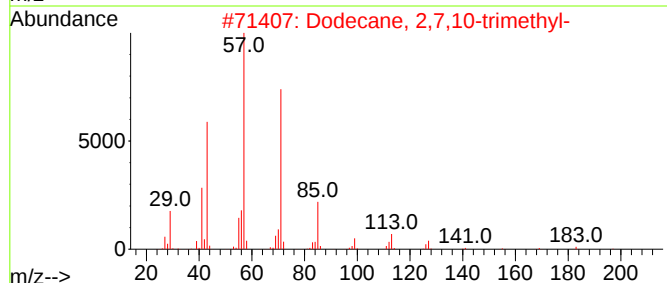
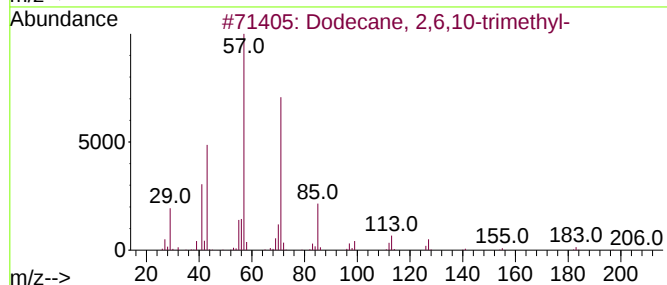
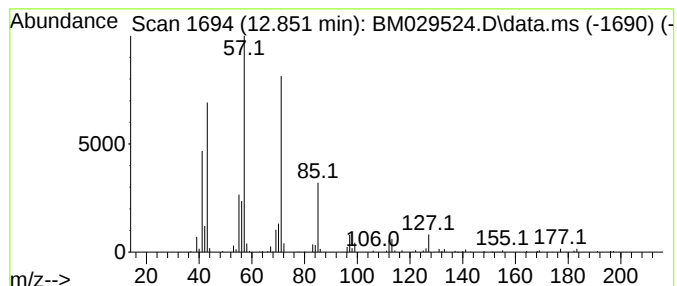
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Dodecane, 2,6,10-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.851	5.19 ng	311909	Acenaphthene-d10		14.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-		212	C15H32	003891-98-3	86
2	Dodecane, 2,7,10-trimethyl-		212	C15H32	074645-98-0	72
3	Undecane, 5-methyl-		170	C12H26	001632-70-8	72
4	Heptadecane, 7-methyl-		254	C18H38	020959-33-5	72
5	Undecane, 2,4-dimethyl-		184	C13H28	017312-80-0	64



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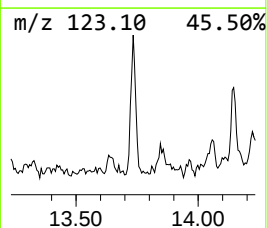
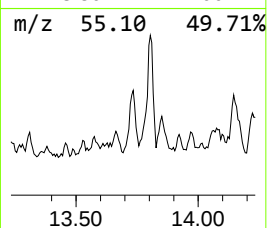
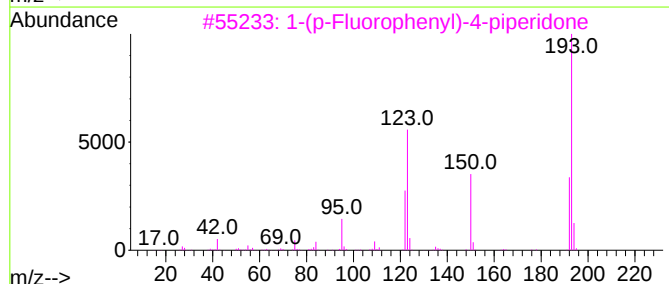
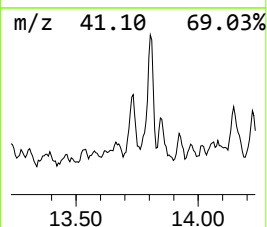
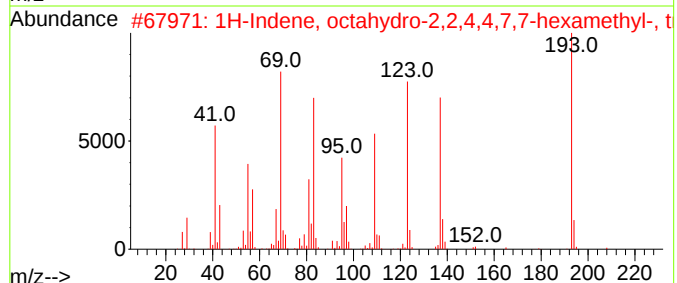
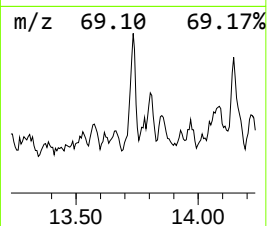
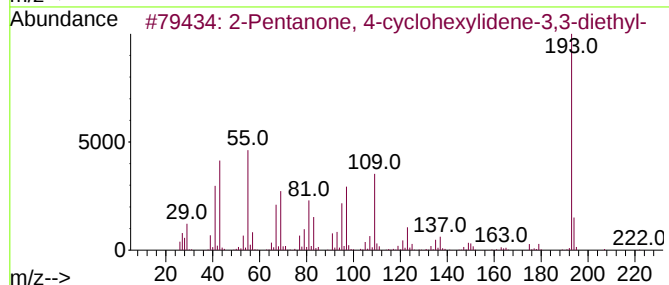
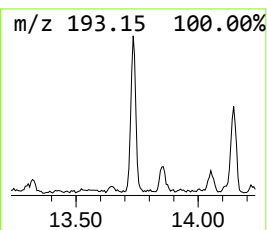
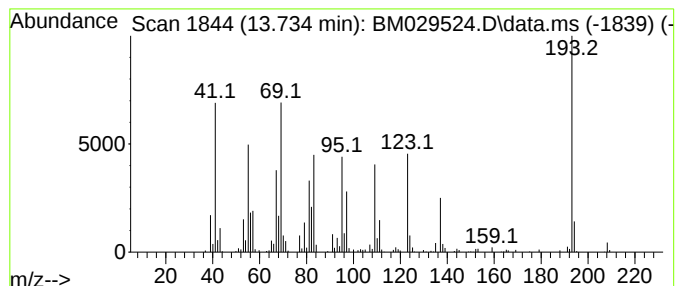
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown13.733 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	4.36 ng	261692	Acenaphthene-d10	14.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	47
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	42
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
4			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	32
5			2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	007056-56-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
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ALS Vial : 11 Sample Multiplier: 1

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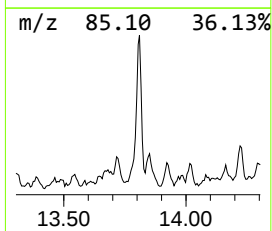
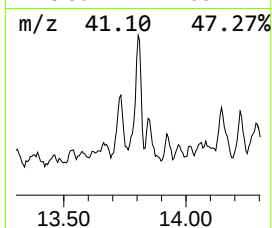
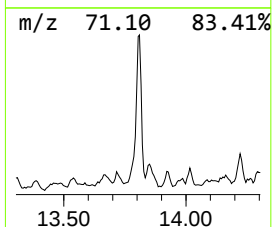
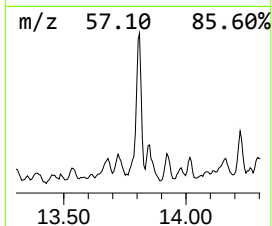
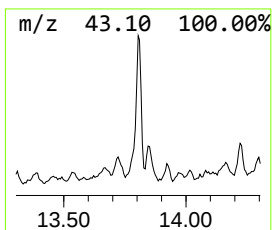
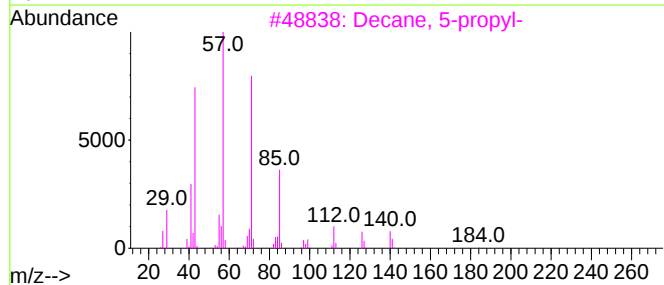
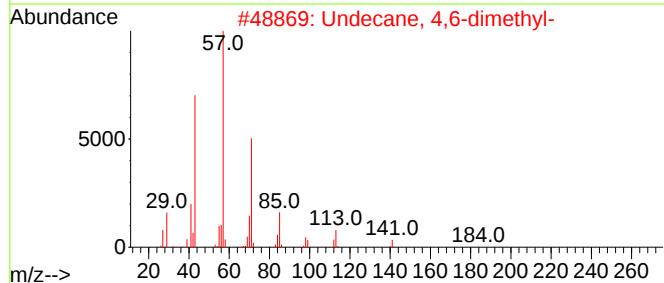
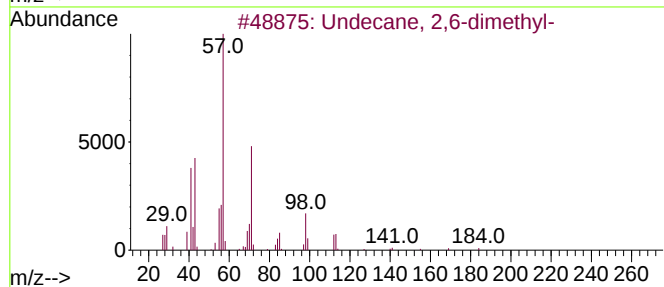
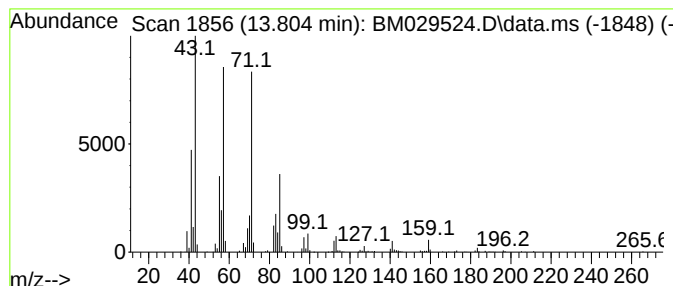
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Undecane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	9.60 ng	576880	Acenaphthene-d10	14.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	80
2			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	74
3			Decane, 5-propyl-	184	C13H28	017312-62-8	72
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	64
5			Hexadecane	226	C16H34	000544-76-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
Operator : CG/JU
Sample : M1998-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-3A

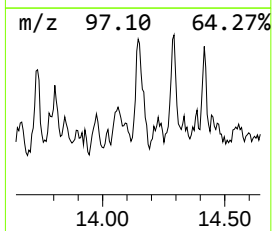
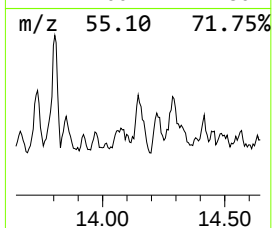
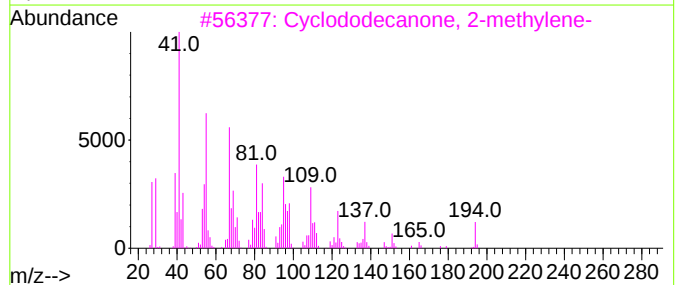
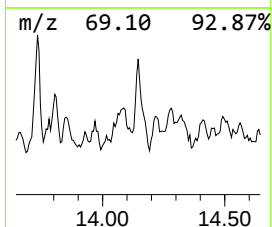
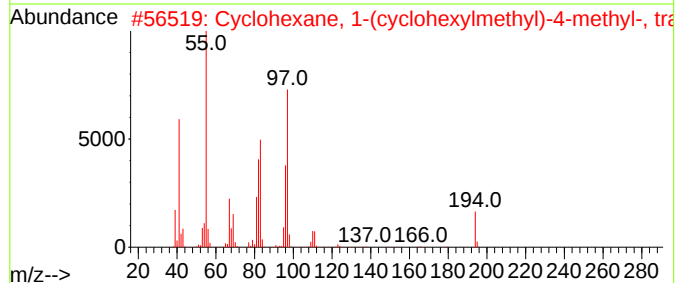
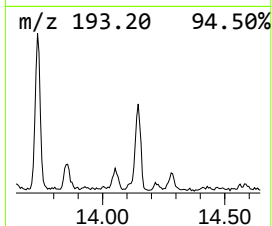
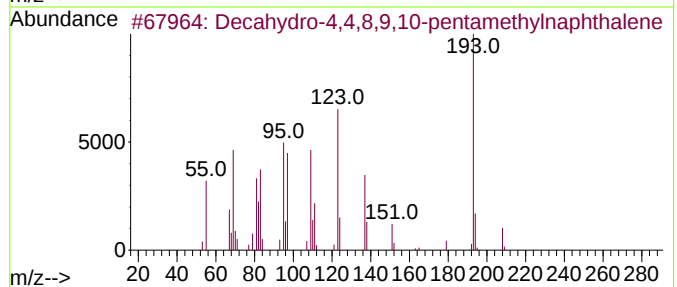
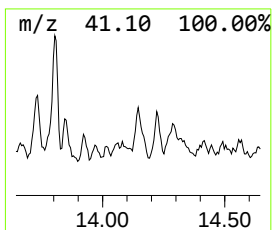
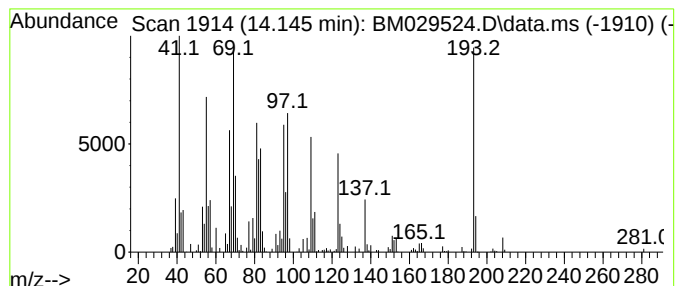
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown14.145 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	4.89 ng	293941	Acenaphthene-d10	14.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
2		Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-98-2	35
3		Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	30
4		(-)-trans-Pinane	138	C10H18	033626-25-4	25
5		7-Pentadecyne	208	C15H28	022089-89-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
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Sample : M1998-01
Misc :
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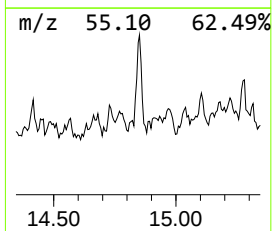
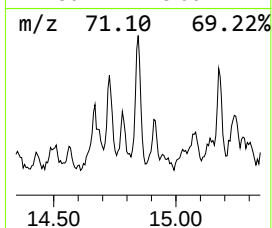
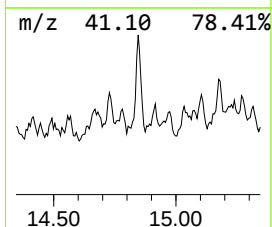
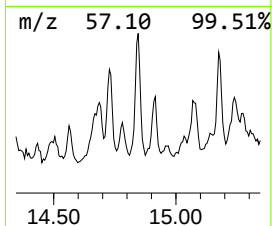
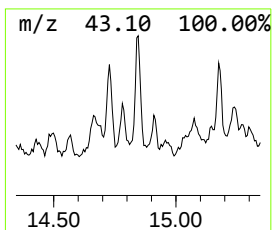
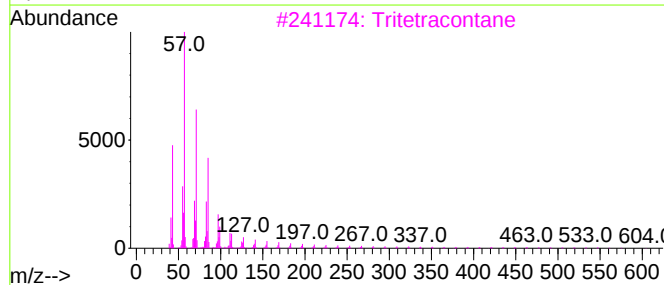
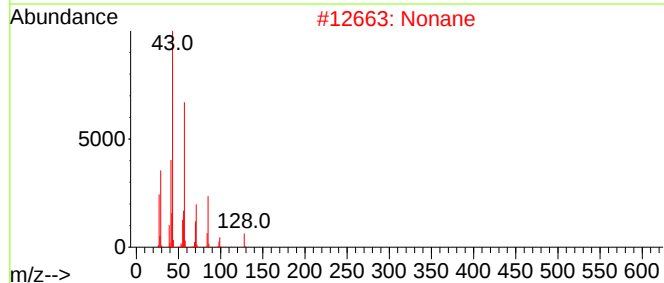
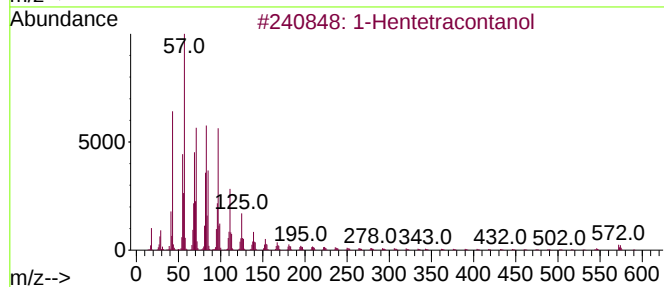
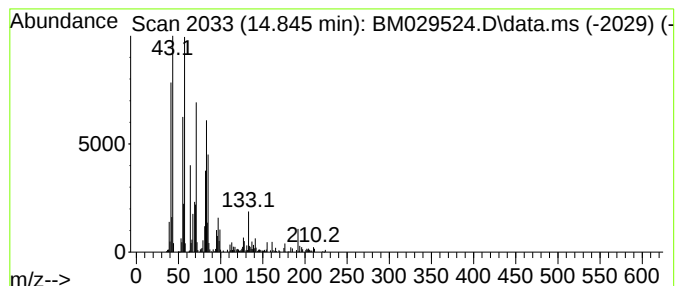
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown14.845 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.845	5.75 ng	345656	Acenaphthene-d10	14.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hentetracontanol	593	C41H84O	040710-42-7	38
2	Nonane	128	C9H20	000111-84-2	25
3	Tritetracontane	605	C43H88	007098-21-7	25
4	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	25
5	Tetratetracontane	619	C44H90	007098-22-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
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Sample : M1998-01
Misc :
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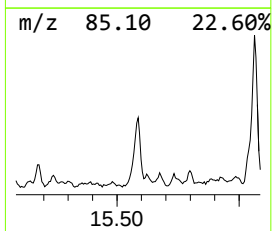
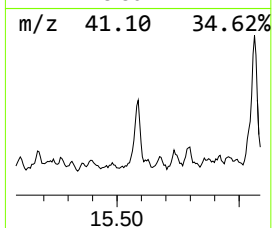
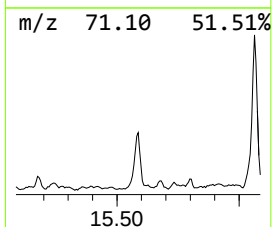
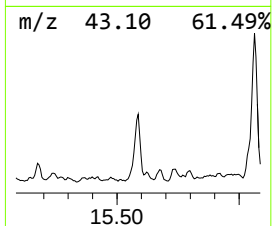
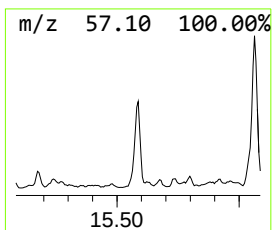
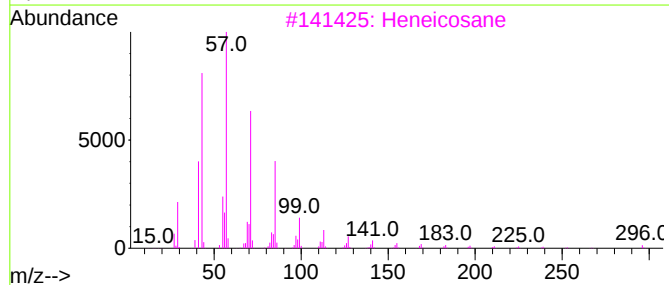
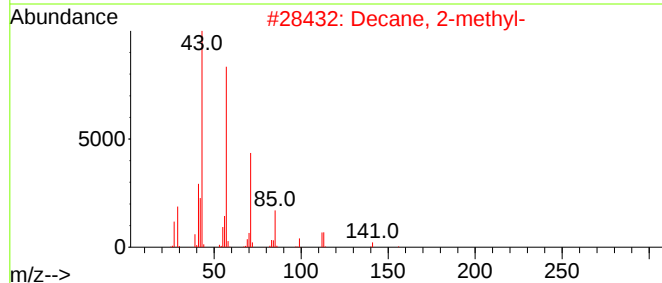
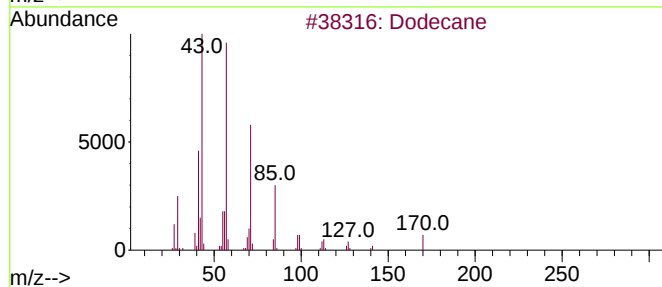
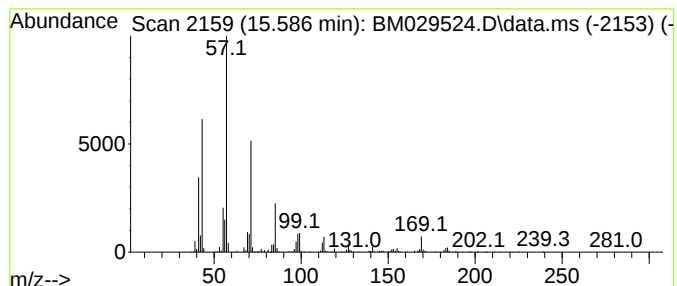
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.586	9.49 ng	570187	Acenaphthene-d10		14.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecane		170	C12H26	000112-40-3	74
2	Decane, 2-methyl-		156	C11H24	006975-98-0	74
3	Heneicosane		296	C21H44	000629-94-7	72
4	Eicosane		282	C20H42	000112-95-8	72
5	Hexadecane		226	C16H34	000544-76-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
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Sample : M1998-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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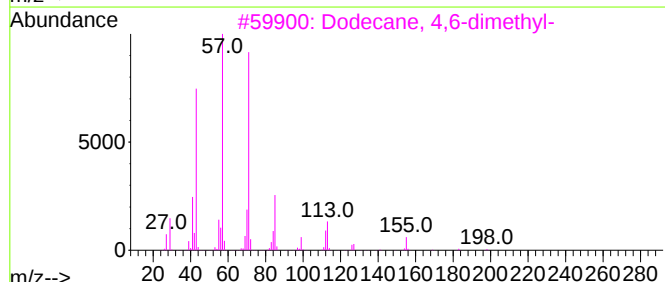
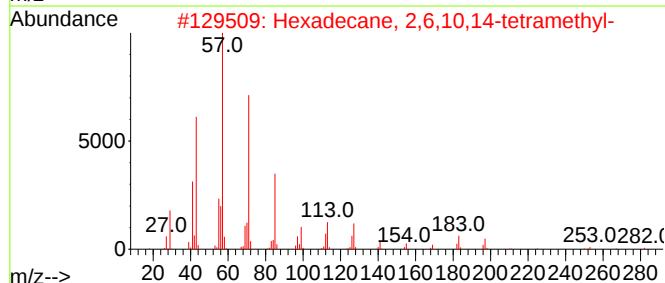
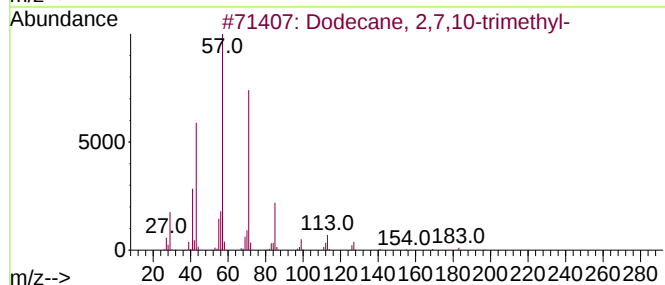
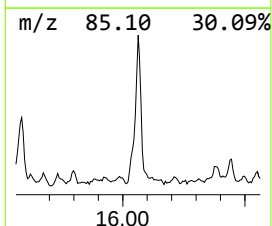
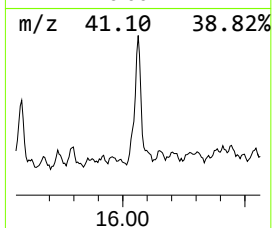
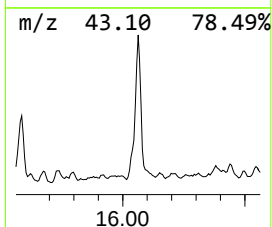
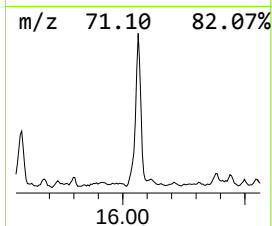
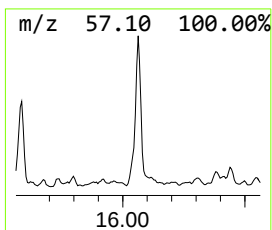
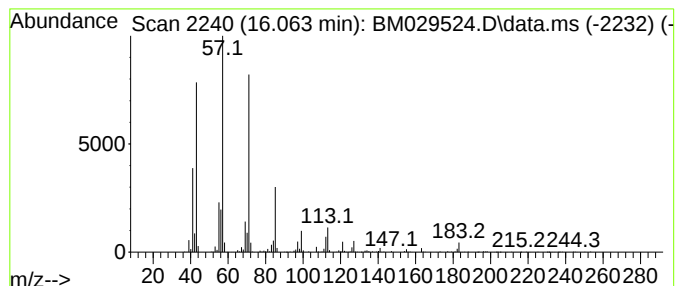
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Dodecane, 2,7,10-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.063	24.66 ng	1419480	Phenanthrene-d10	17.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	91
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
3		Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	83
4		Decane, 2-methyl-	156	C11H24	006975-98-0	83
5		Tridecane, 5-propyl-	226	C16H34	055045-11-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
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Sample : M1998-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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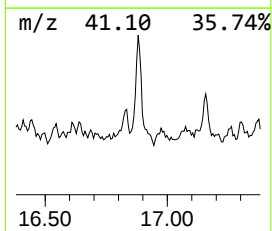
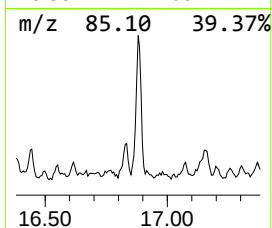
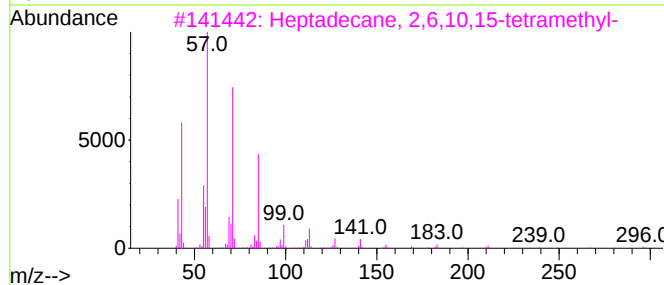
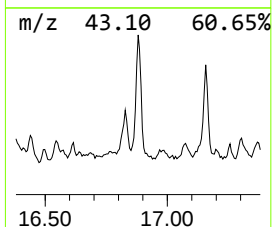
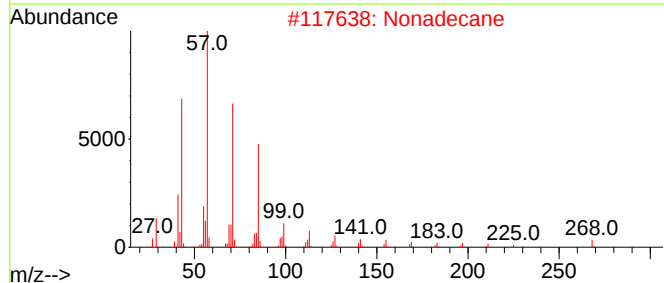
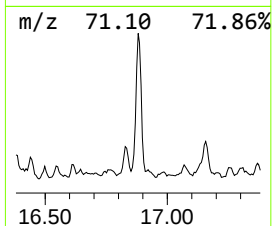
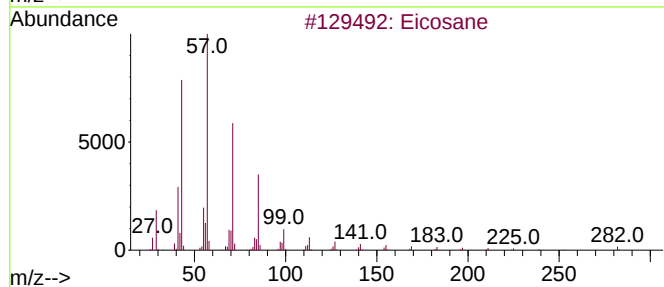
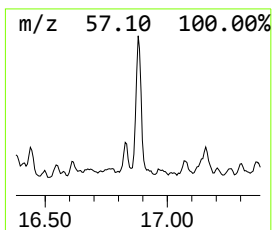
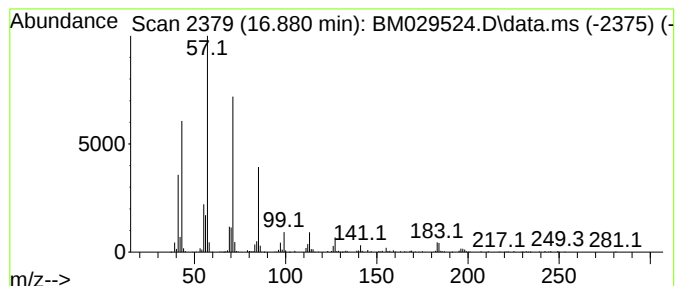
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.880	12.35 ng	711133	Phenanthrene-d10	17.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	86
2		Nonadecane	268	C19H40	000629-92-5	86
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4		Tetracosane	338	C24H50	000646-31-1	86
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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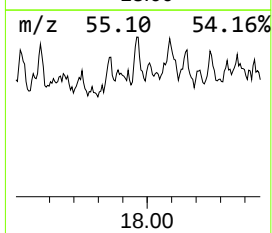
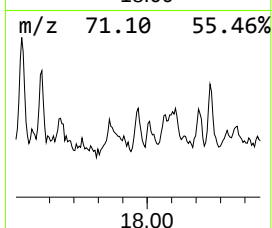
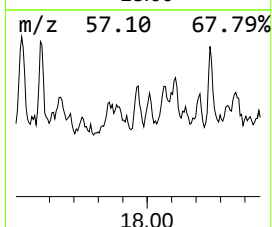
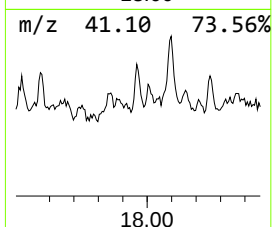
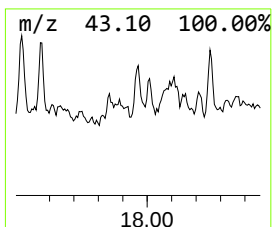
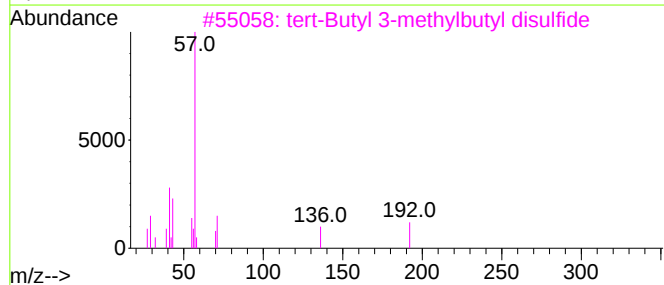
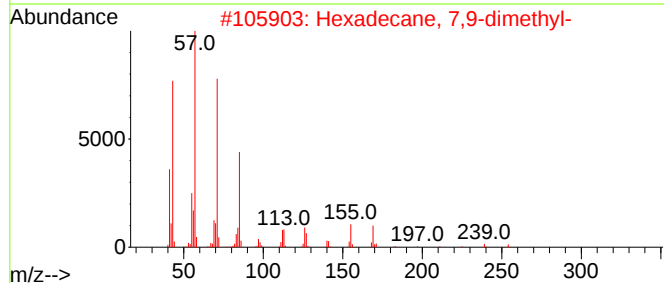
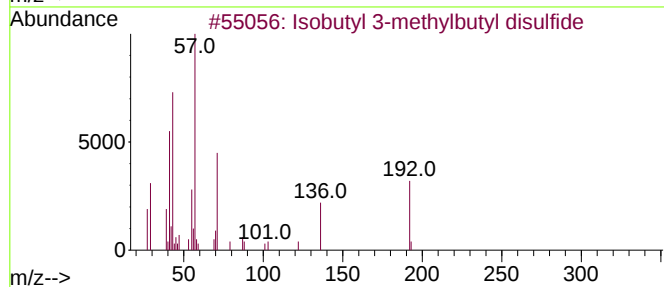
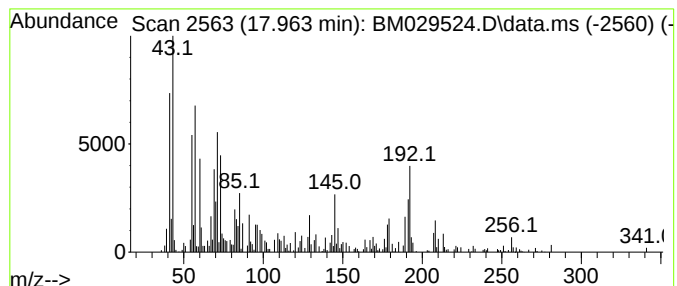
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown17.963 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.963	3.86 ng	222053	Phenanthrene-d10	17.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutyl 3-methylbutyl disulfide	192	C9H20S2	075203-66-6	25
2		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	25
3		tert-Butyl 3-methylbutyl disulfide	192	C9H20S2	075203-68-8	22
4		Dodecane	170	C12H26	000112-40-3	15
5		1-Threitol, 2-O-nonyl-	248	C13H28O4	163776-15-6	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
Operator : CG/JU
Sample : M1998-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-3A

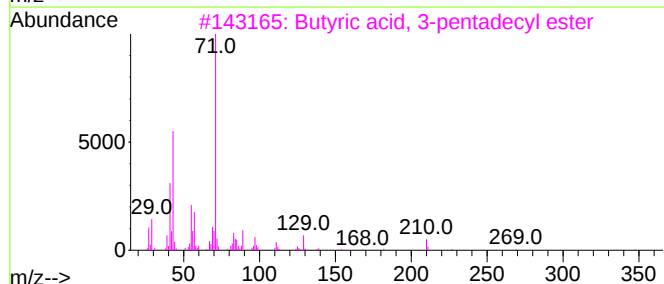
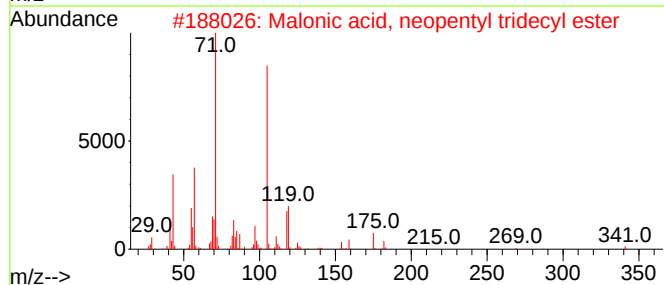
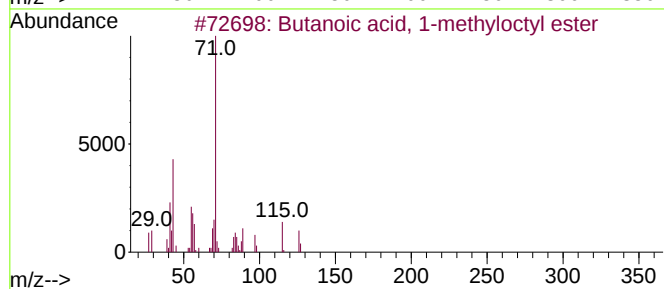
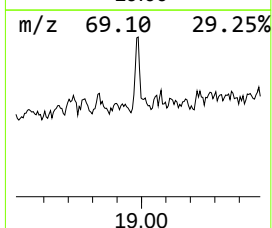
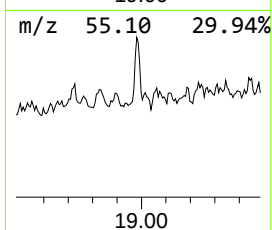
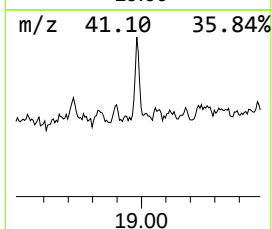
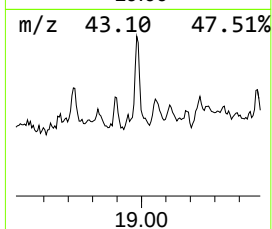
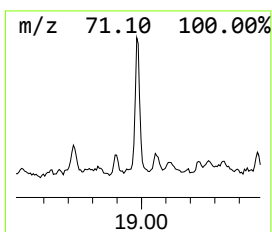
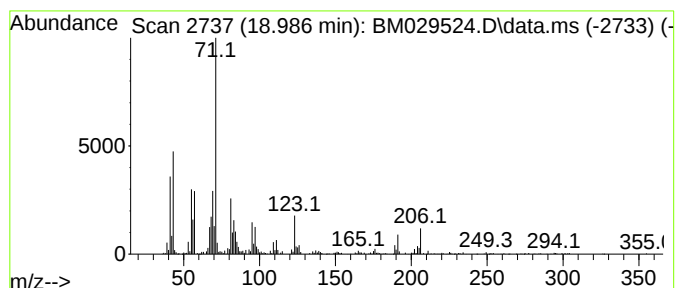
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Butanoic acid, 1-methylocty... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.986	6.82 ng	392712	Phenanthrene-d10	17.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	50
2			Malonic acid, neopentyl tridecyl...	356	C21H40O4	1000363-93-6	50
3			Butyric acid, 3-pentadecyl ester	298	C19H38O2	1000280-57-3	50
4			Nonane, 5-butyl-	184	C13H28	017312-63-9	50
5			2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
Operator : CG/JU
Sample : M1998-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-3A

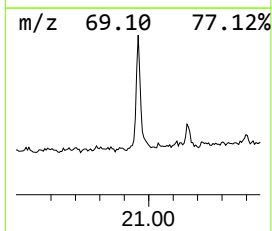
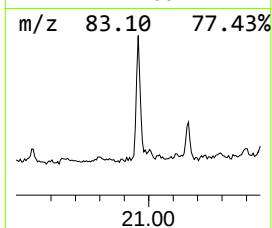
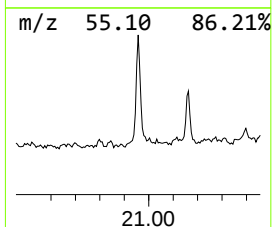
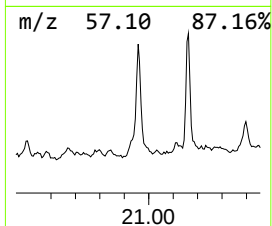
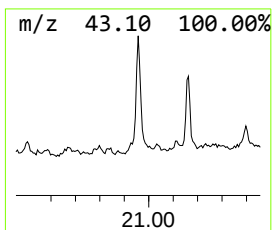
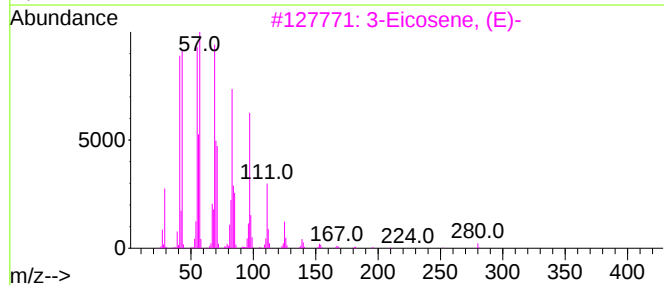
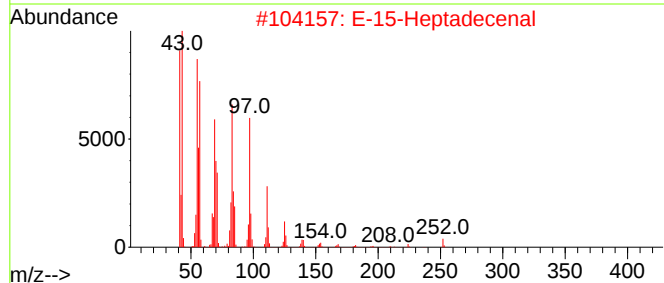
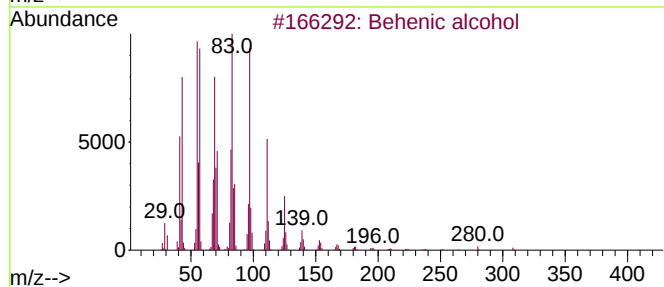
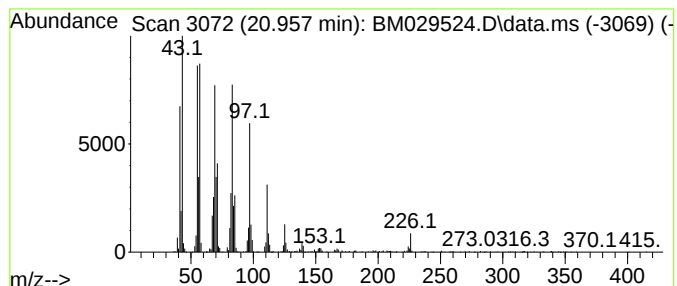
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	14.72 ng	1058630	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			E-15-Heptadecenal	252	C17H32O	1000130-97-9	93
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
Data File : BM029524.D
Acq On : 16 Apr 2021 16:31
Operator : CG/JU
Sample : M1998-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

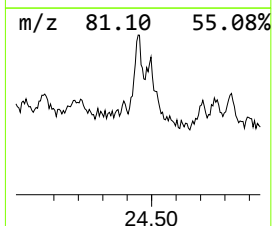
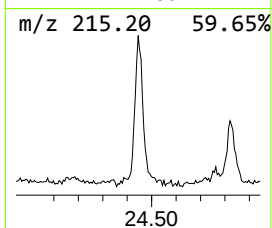
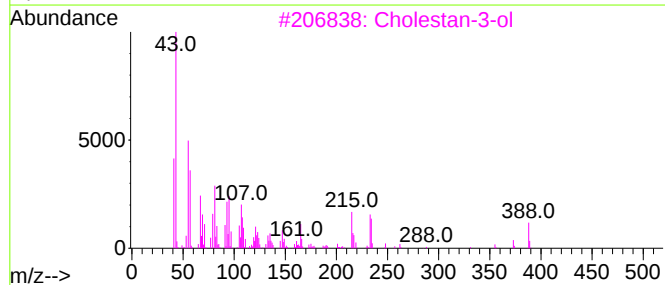
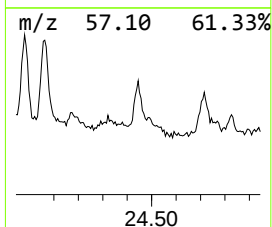
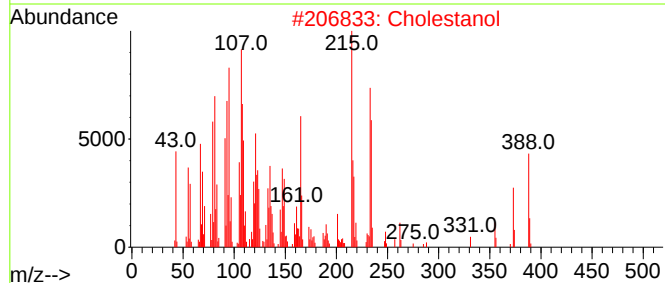
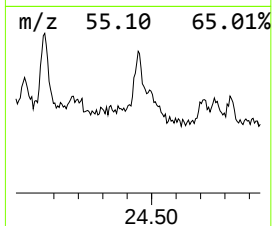
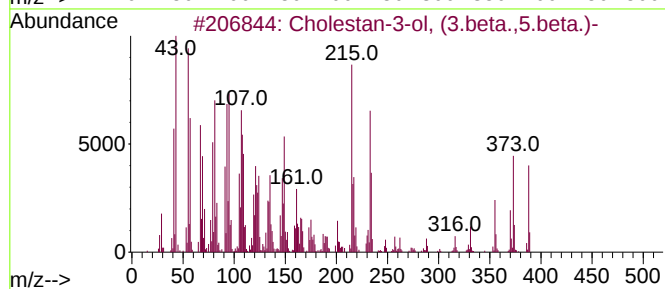
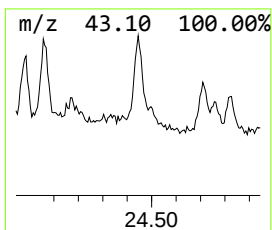
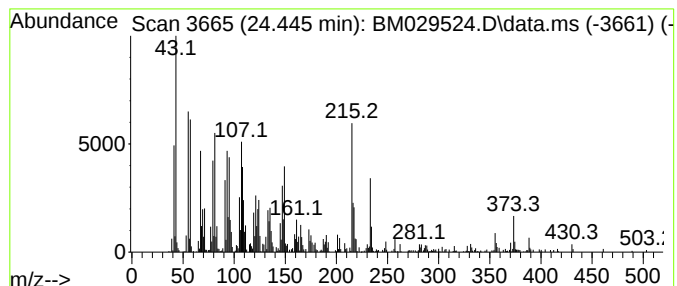
Instrument :
BNA_M
ClientSampleId :
SB-3A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Cholestan-3-ol, (3.beta.,5.... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.445	8.55 ng	513699	Perylene-d12	23.445	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	78
2	Cholestanol	388	C27H48O	000080-97-7	72
3	Cholestan-3-ol	388	C27H48O	027409-41-2	64
4	Methyl lithocholate	390	C25H42O3	001249-75-8	55
5	Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	062337-99-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
 Data File : BM029524.D
 Acq On : 16 Apr 2021 16:31
 Operator : CG/JU
 Sample : M1998-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-3A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.922	35.5	ng	1119970	1	7.675	630340	20.0
2-Pentanone, 4-...	4.816	9.6	ng	301120	1	7.675	630340	20.0
Heptane, 2,2,6,...	7.310	3.9	ng	121369	1	7.675	630340	20.0
3-Heptene, 2,2,...	7.463	4.8	ng	151749	1	7.675	630340	20.0
2-Piperidinone	10.198	5.4	ng	237028	2	10.451	878657	20.0
Octane, 2,6-dim...	11.487	7.2	ng	315511	2	10.451	878657	20.0
Indole	11.951	5.1	ng	222267	2	10.451	878657	20.0
Decane, 2,3,5-t...	12.116	5.3	ng	233115	2	10.451	878657	20.0
Dodecane, 2,6,1...	12.851	5.2	ng	311909	3	14.310	1201650	20.0
unknown13.733	13.733	4.4	ng	261692	3	14.310	1201650	20.0
Undecane, 2,6-d...	13.804	9.6	ng	576880	3	14.310	1201650	20.0
unknown14.145	14.145	4.9	ng	293941	3	14.310	1201650	20.0
unknown14.845	14.845	5.8	ng	345656	3	14.310	1201650	20.0
Dodecane	15.586	9.5	ng	570187	3	14.310	1201650	20.0
Dodecane, 2,7,1...	16.063	24.7	ng	1419480	4	17.057	1151290	20.0
Eicosane	16.880	12.4	ng	711133	4	17.057	1151290	20.0
unknown17.963	17.963	3.9	ng	222053	4	17.057	1151290	20.0
Butanoic acid, ...	18.986	6.8	ng	392712	4	17.057	1151290	20.0
Behenic alcohol	20.957	14.7	ng	1058630	5	21.233	1437890	20.0
Cholestan-3-ol,...	24.445	8.6	ng	513699	6	23.445	1201750	20.0