

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
 Data File : BP013457.D
 Acq On : 11 Jan 2023 22:45
 Operator : CG/JU
 Sample : 01064-07 10X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-14-02

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-BP121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013457.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.223	3	6	21	rVB	3804965	5752760	7.31%	1.001%
2	3.846	107	112	127	rBV	1693947	3127009	3.98%	0.544%
3	3.964	127	132	146	rVB2	1324422	2417838	3.07%	0.421%
4	4.446	203	214	249	rBV	29551200	68435259	87.00%	11.904%
5	5.399	367	376	383	rBV	2808779	5881630	7.48%	1.023%
6	5.752	429	436	442	rBV	797217	1524779	1.94%	0.265%
7	5.846	447	452	461	rVV	1826455	2999244	3.81%	0.522%
8	5.964	466	472	477	rVV	1764841	3305245	4.20%	0.575%
9	6.011	477	480	491	rVB	580438	992238	1.26%	0.173%
10	6.869	620	626	633	rBV2	2795153	4426288	5.63%	0.770%
11	7.022	635	652	653	rBV2	1544807	4813424	6.12%	0.837%
12	7.099	661	665	667	rBV2	649303	1102213	1.40%	0.192%
13	7.252	687	691	696	rVB	607162	875562	1.11%	0.152%
14	7.405	712	717	723	rVB	2926779	4165037	5.29%	0.725%
15	7.611	744	752	759	rVV	1331555	2217347	2.82%	0.386%
16	7.775	772	780	792	rVB2	522157	1255424	1.60%	0.218%
17	7.922	794	805	812	rBV	1757140	2714921	3.45%	0.472%
18	8.169	839	847	853	rBV2	623486	1622558	2.06%	0.282%
19	8.316	862	872	883	rBV3	1073074	2394621	3.04%	0.417%
20	8.475	892	899	903	rBV	1067198	2122621	2.70%	0.369%
21	8.540	903	910	920	rVB3	5121855	12725593	16.18%	2.214%
22	8.663	926	931	943	rVB2	757149	1542760	1.96%	0.268%
23	8.799	949	954	958	rBV	819787	1520811	1.93%	0.265%
24	9.087	996	1003	1006	rBV	9928509	16299417	20.72%	2.835%
25	9.116	1006	1008	1015	rVB	4490830	6243493	7.94%	1.086%
26	9.252	1024	1031	1041	rVB2	3530978	6650141	8.45%	1.157%
27	9.799	1115	1124	1132	rVB	635939	1482722	1.88%	0.258%
28	9.916	1139	1144	1150	rVV	2478282	4230628	5.38%	0.736%
29	9.969	1150	1153	1162	rVB2	492189	919908	1.17%	0.160%
30	10.105	1169	1176	1179	rVV	1304109	2715261	3.45%	0.472%
31	10.693	1265	1276	1280	rBV6	1321467	4137524	5.26%	0.720%
32	10.734	1280	1283	1293	rVB	2737293	4525710	5.75%	0.787%
33	10.822	1293	1298	1307	rVB	547480	975258	1.24%	0.170%
34	11.022	1326	1332	1337	rVB	1027069	1575381	2.00%	0.274%
35	11.140	1349	1352	1367	rVB3	379272	956079	1.22%	0.166%
36	11.316	1376	1382	1386	rBV	538969	1025851	1.30%	0.178%

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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 >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.416	1390	1399	1405	rVV	12631697	21535116	27.38%	3.746%
38	11.469	1405	1408	1413	rVV3	505670	940647	1.20%	0.164%
39	11.522	1413	1417	1420	rVV	1255813	2074064	2.64%	0.361%
40	11.575	1420	1426	1432	rVV2	1973325	4043990	5.14%	0.703%
41	11.675	1432	1443	1448	rVV2	4372013	9328627	11.86%	1.623%
42	11.722	1448	1451	1461	rVB3	694981	1272809	1.62%	0.221%
43	11.946	1485	1489	1498	rVB	532498	995962	1.27%	0.173%
44	12.087	1508	1513	1517	rBV	520338	874300	1.11%	0.152%
45	12.146	1517	1523	1532	rVB	6114473	9736135	12.38%	1.694%
46	12.228	1532	1537	1542	rVB	666575	960716	1.22%	0.167%
47	12.381	1551	1563	1571	rBV5	731319	1868063	2.37%	0.325%
48	12.475	1572	1579	1585	rBV	13837583	20671959	26.28%	3.596%
49	12.540	1585	1590	1599	rVB5	477991	1288811	1.64%	0.224%
50	12.775	1623	1630	1634	rBV	6598197	10712341	13.62%	1.863%
51	12.846	1634	1642	1650	rVV	15694511	29343171	37.30%	5.104%
52	13.022	1667	1672	1686	rVB2	6405789	11575137	14.71%	2.014%
53	13.134	1687	1691	1696	rBV	1102535	1516298	1.93%	0.264%
54	13.210	1696	1704	1712	rVB2	3391676	6187089	7.87%	1.076%
55	13.287	1712	1717	1721	rBV	1114714	1813907	2.31%	0.316%
56	13.593	1760	1769	1776	rVB	4399315	8499507	10.80%	1.479%
57	13.757	1788	1797	1801	rBV3	744097	1584817	2.01%	0.276%
58	14.122	1853	1859	1863	rBV4	746298	1450609	1.84%	0.252%
59	14.193	1863	1871	1875	rBV2	4512624	8184753	10.40%	1.424%
60	14.369	1891	1901	1906	rBV2	4305298	9447315	12.01%	1.643%
61	14.493	1918	1922	1929	rVB	537565	859305	1.09%	0.149%
62	14.569	1929	1935	1941	rBV	4501209	6630316	8.43%	1.153%
63	14.628	1941	1945	1951	rVB	778802	1100618	1.40%	0.191%
64	15.069	2016	2020	2025	rBV3	744524	995138	1.27%	0.173%
65	15.240	2045	2049	2056	rVB3	535711	872244	1.11%	0.152%
66	15.563	2097	2104	2106	rBV5	540353	991160	1.26%	0.172%
67	15.598	2106	2110	2119	rVB2	854207	1601503	2.04%	0.279%
68	15.722	2127	2131	2135	rBV2	804394	1051182	1.34%	0.183%
69	15.928	2161	2166	2173	rBV	586918	1096901	1.39%	0.191%
70	16.069	2185	2190	2195	rBV2	1382124	2169071	2.76%	0.377%
71	17.328	2399	2404	2412	rBV	6687787	9981846	12.69%	1.736%
72	17.686	2461	2465	2477	rVB2	607003	1057645	1.34%	0.184%
73	18.222	2548	2556	2584	rVV	25846332	61620014	78.33%	10.719%
74	18.945	2676	2679	2688	rBV	927981	1474526	1.87%	0.256%
75	19.216	2719	2725	2729	rBV2	1822978	2851530	3.62%	0.496%
76	19.345	2734	2747	2756	rBV	27798378	78663466	100.00%	13.684%

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 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	19.445	2761	2764	2781	rVB	10625774	16648235	21.16%	2.896%
78	19.880	2834	2838	2841	rBV	2761899	3247638	4.13%	0.565%
79	19.933	2844	2847	2855	rVB2	1857319	2949143	3.75%	0.513%
80	20.175	2885	2888	2892	rBV	1890180	2433862	3.09%	0.423%
81	20.216	2893	2895	2900	rVB	1534750	1675468	2.13%	0.291%
82	20.557	2951	2953	2957	rVB	1380191	1413961	1.80%	0.246%
83	21.045	3033	3036	3040	rVB2	2261215	2461000	3.13%	0.428%
84	21.416	3095	3099	3105	rBV	6831253	9300046	11.82%	1.618%
85	23.886	3516	3519	3527	rVB2	3470308	6144388	7.81%	1.069%

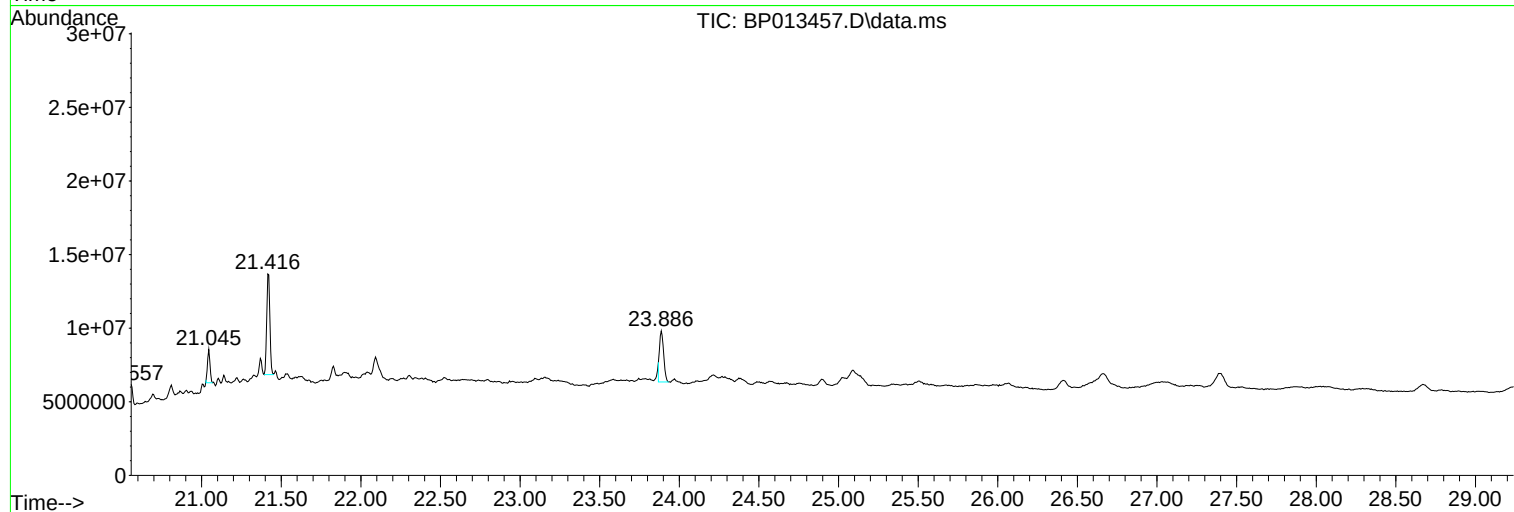
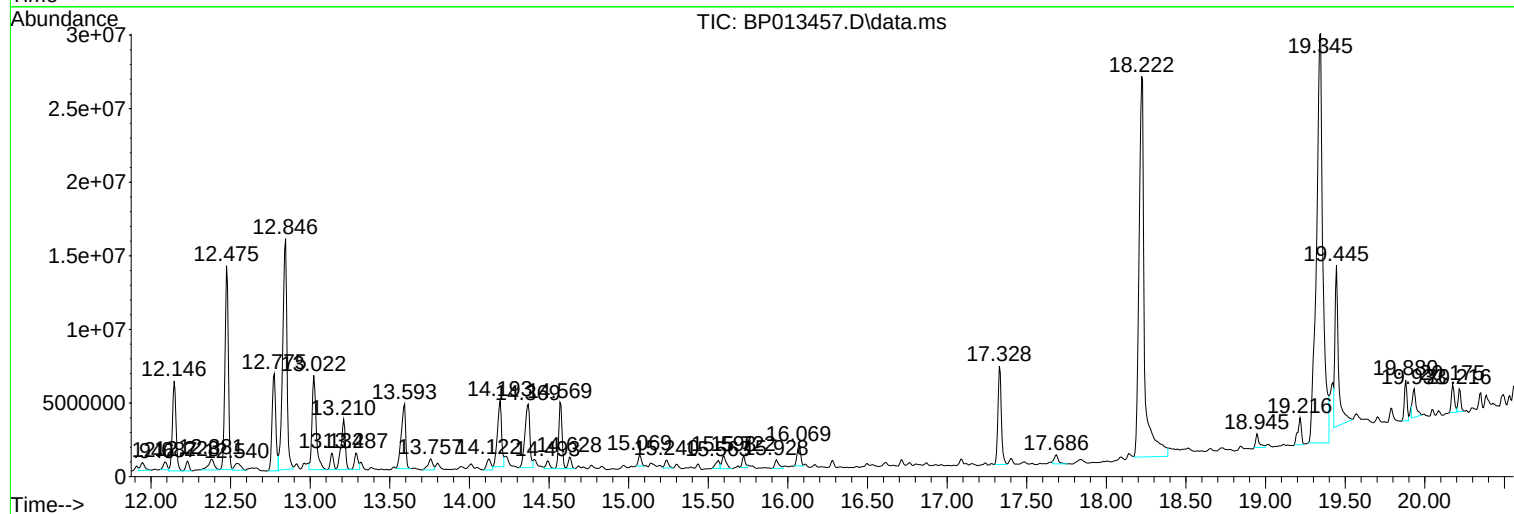
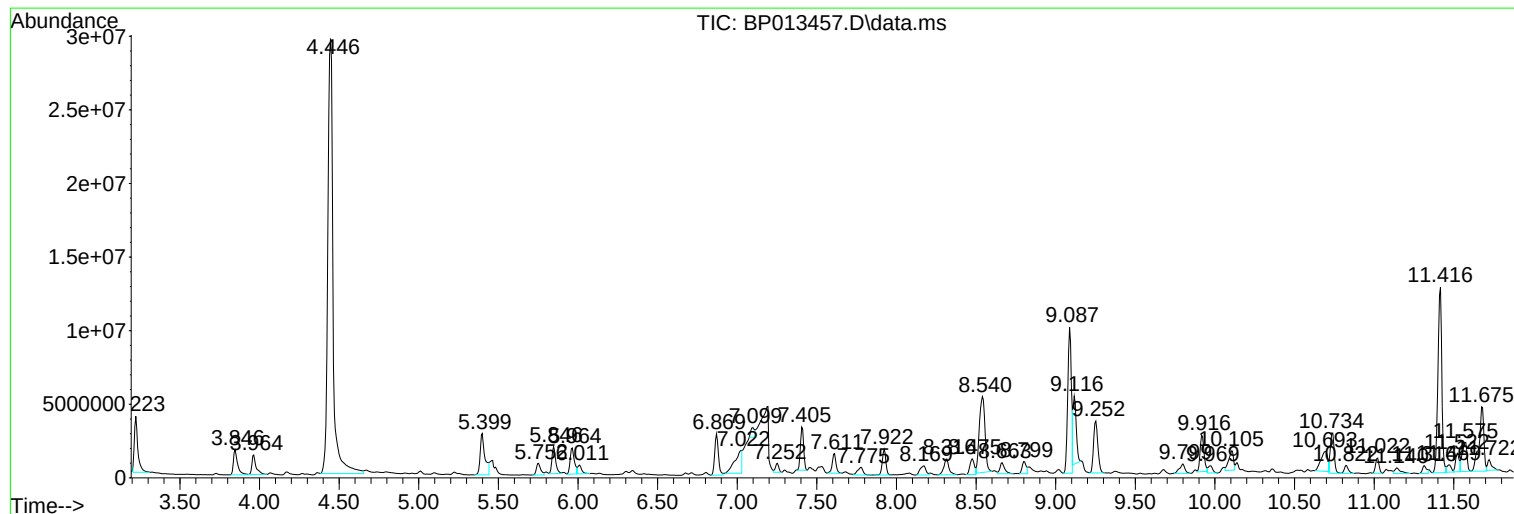
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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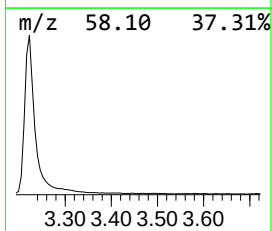
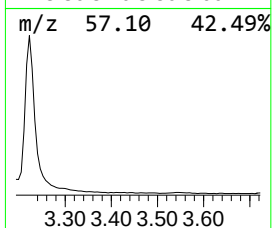
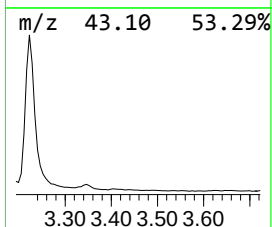
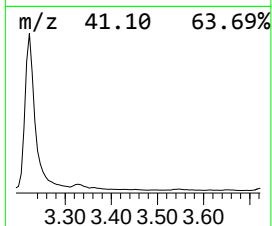
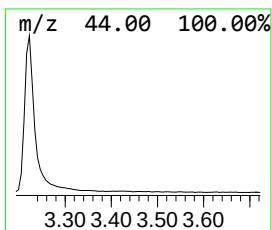
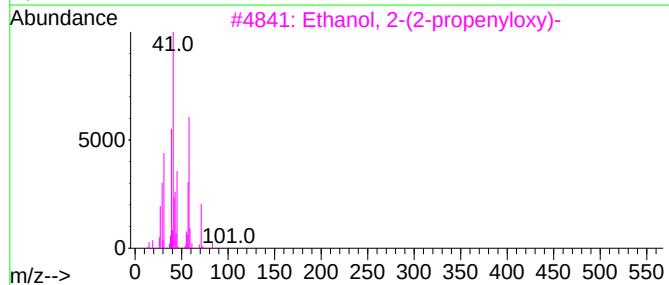
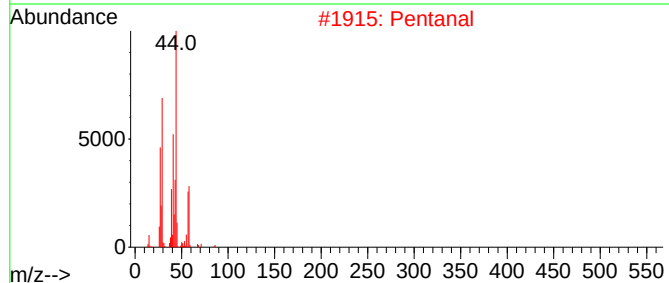
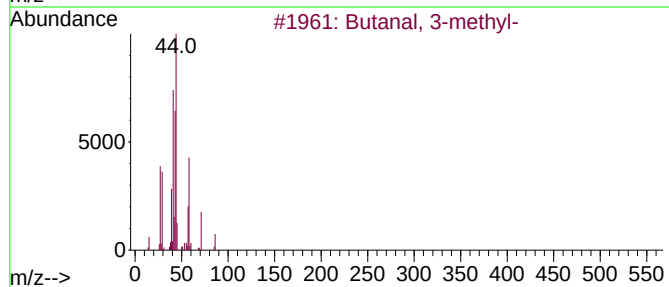
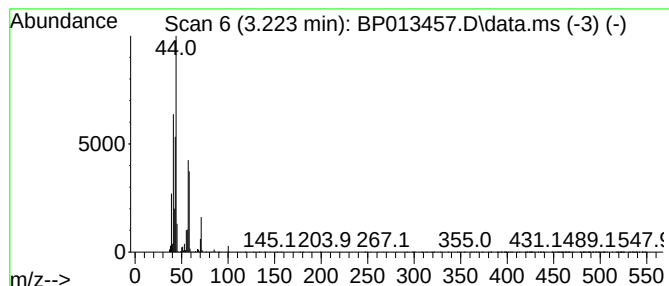
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanal, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.223	42.38 ng	5752760	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
2			Pentanal	86	C5H10O	000110-62-3	59
3			Ethanol, 2-(2-propenyloxy)-	102	C5H10O2	000111-45-5	12
4			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	9
5			1-Sec-butyldiaziridine	100	C5H12N2	033657-34-0	9



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Instrument :
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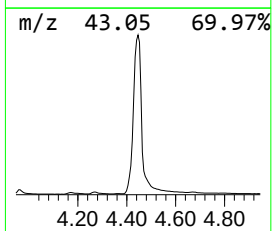
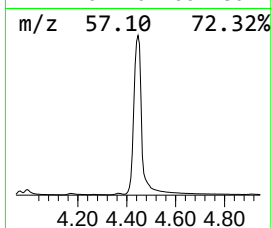
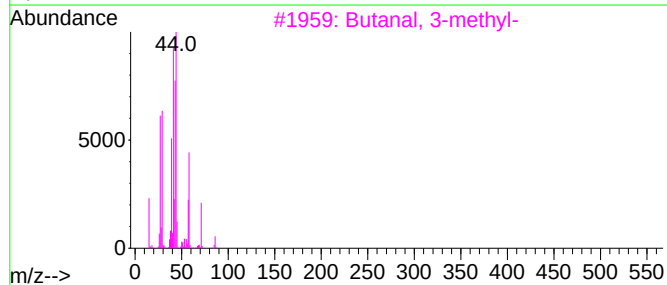
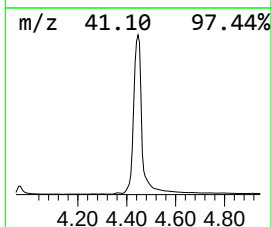
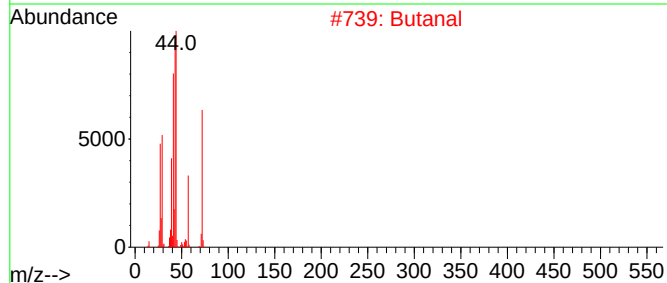
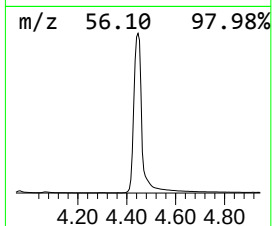
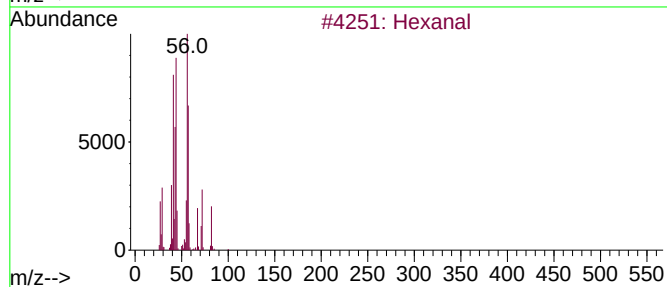
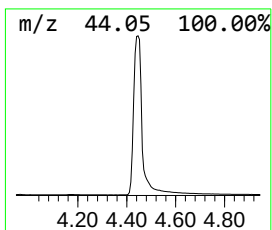
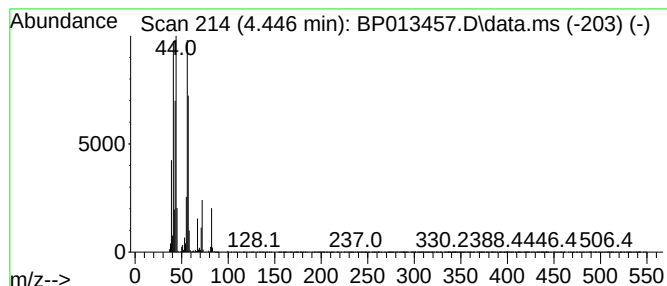
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.446	504.14 ng	68435300	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Butanal			72	C4H8O	000123-72-8	38
3	Butanal, 3-methyl-			86	C5H10O	000590-86-3	32
4	1-Butanol, 2-methyl-, (S)-			88	C5H12O	001565-80-6	22
5	Glutaraldehyde			100	C5H8O2	000111-30-8	14



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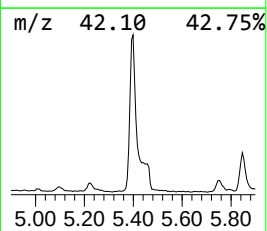
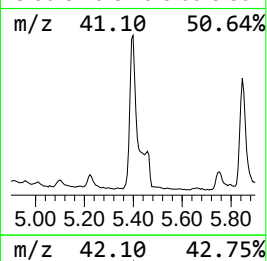
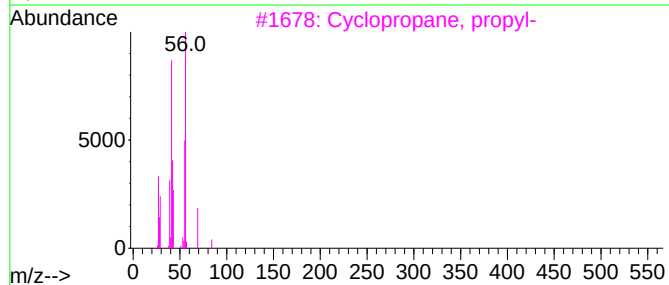
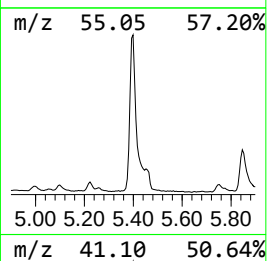
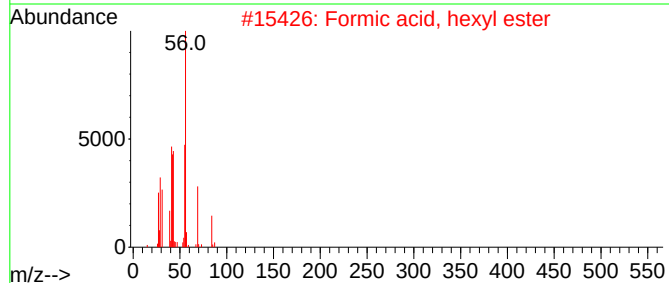
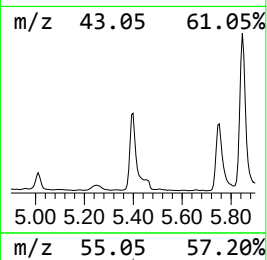
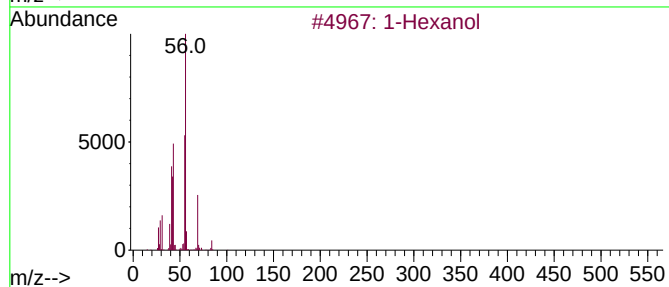
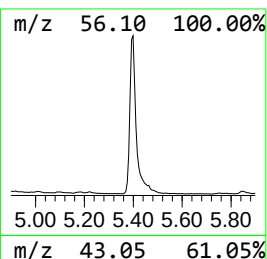
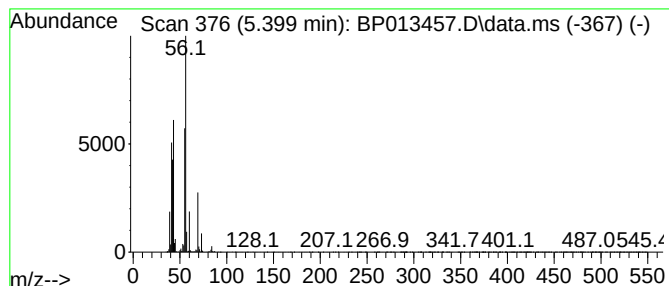
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Hexanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.399	43.33 ng	5881630	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol	102	C6H14O	000111-27-3	72
2			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
3			Cyclopropane, propyl-	84	C6H12	002415-72-7	59
4			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	56
5			1-Butanol	74	C4H10O	000071-36-3	53



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S-14-02

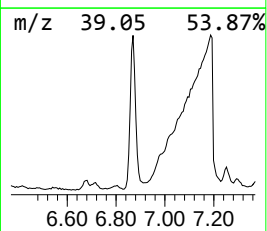
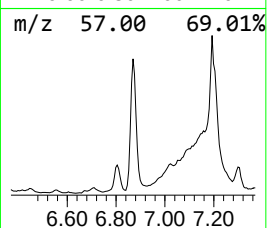
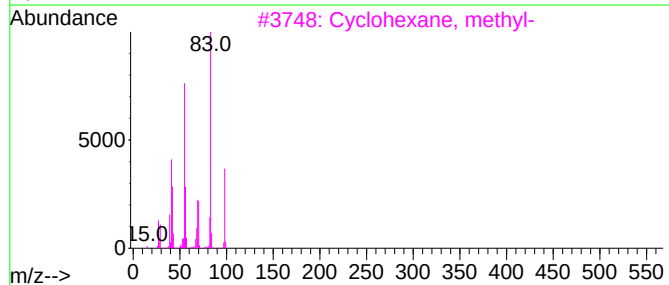
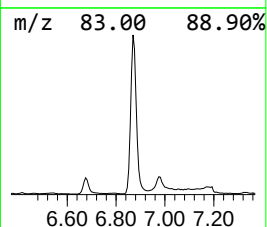
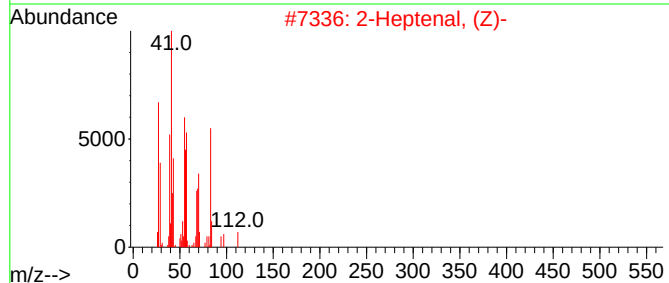
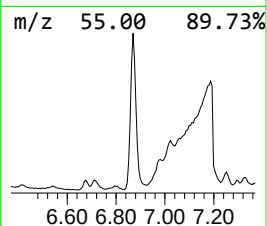
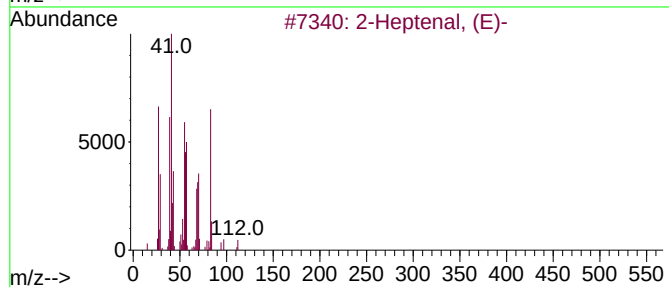
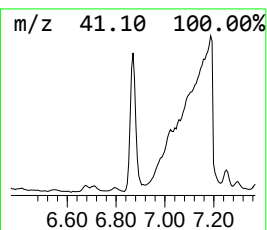
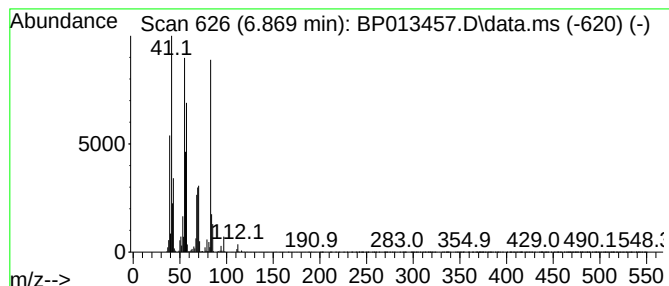
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Heptenal, (E)- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.869	32.61 ng	4426290	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptenal, (E)-	112	C7H12O	018829-55-5	76
2			2-Heptenal, (Z)-	112	C7H12O	057266-86-1	58
3			Cyclohexane, methyl-	98	C7H14	000108-87-2	53
4			3-Ethylcyclopentanone	112	C7H12O	010264-55-8	53
5			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-14-02

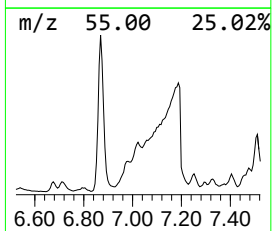
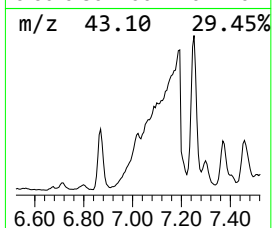
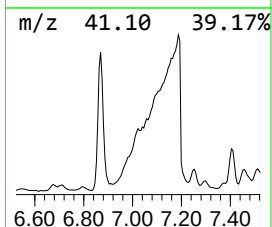
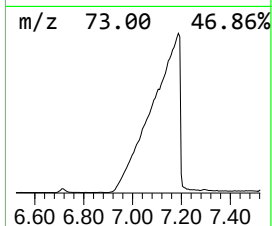
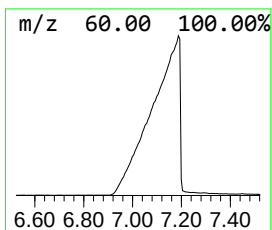
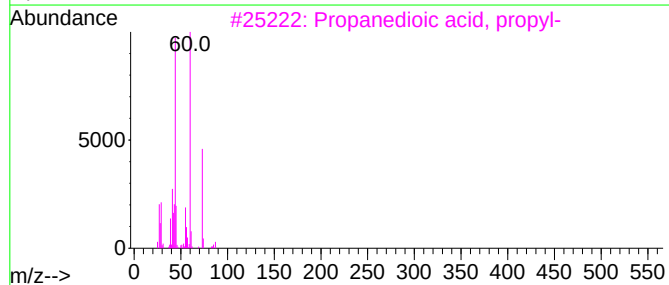
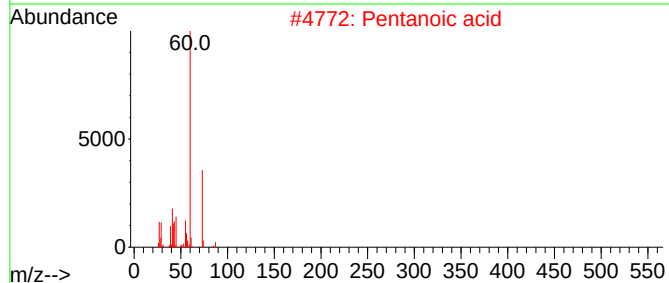
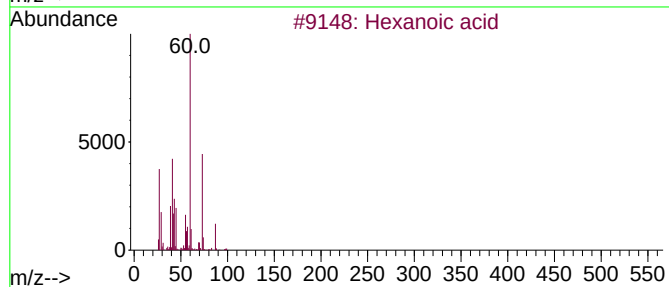
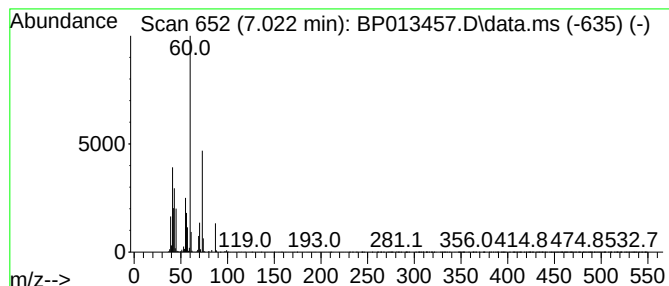
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.022	35.46 ng	4813420	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	78
2			Pentanoic acid	102	C5H10O2	000109-52-4	59
3			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	56
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	42
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
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Instrument :
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ClientSampleId :
S-14-02

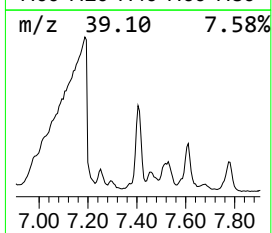
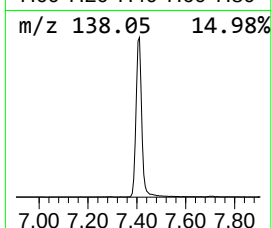
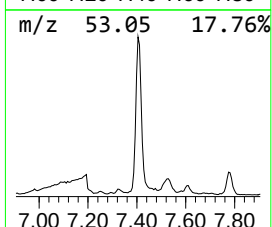
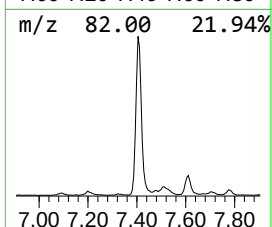
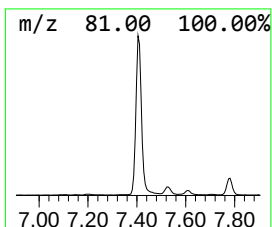
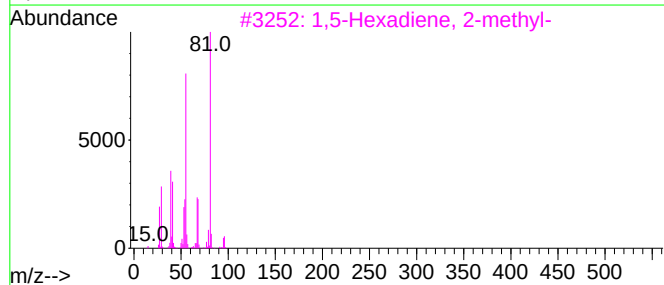
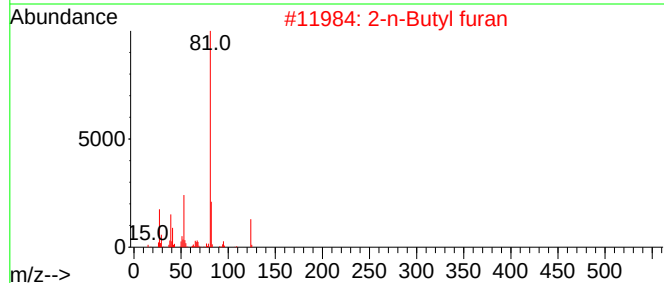
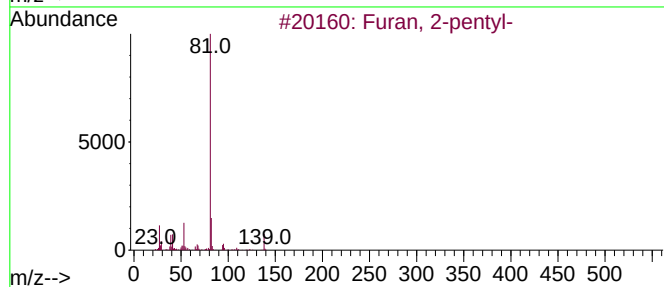
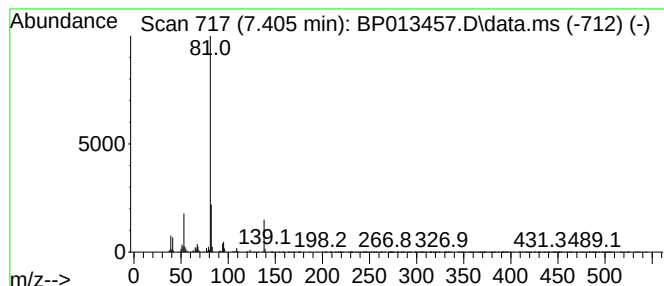
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Furan, 2-pentyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.405	30.68 ng	4165040	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-pentyl-	138	C9H14O	003777-69-3	91
2			2-n-Butyl furan	124	C8H12O	004466-24-4	64
3			1,5-Hexadiene, 2-methyl-	96	C7H12	004049-81-4	36
4			Furan, 2-propyl-	110	C7H10O	004229-91-8	33
5			Ethanone, 1-(2-methyl-2-cyclopentyl)-	124	C8H12O	001767-84-6	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

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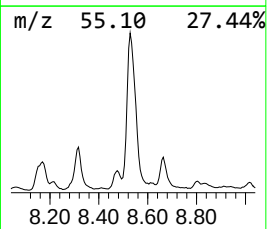
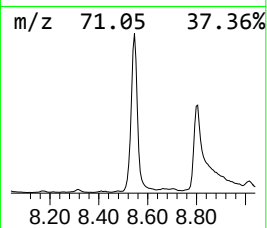
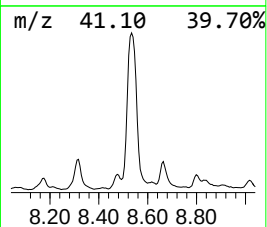
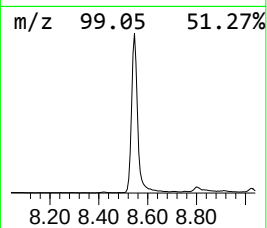
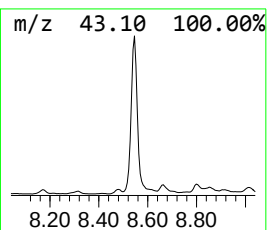
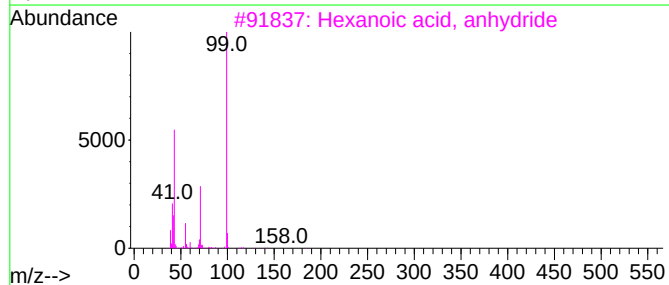
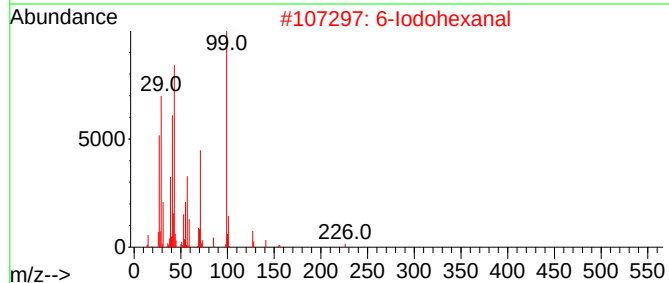
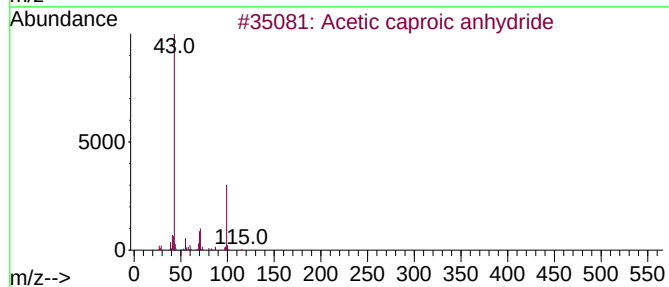
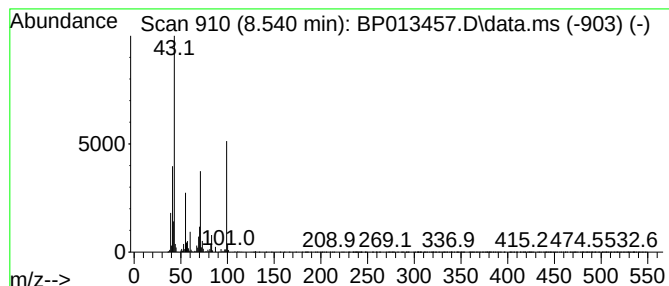
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Acetic caproic anhydride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.540	93.75 ng	12725600	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic caproic anhydride	158	C8H14O3	092351-84-3	64
2			6-Iodohexanal	226	C6H11IO	1000411-49-9	64
3			Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	59
4			n-Caproic acid vinyl ester	142	C8H14O2	003050-69-9	53
5			4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

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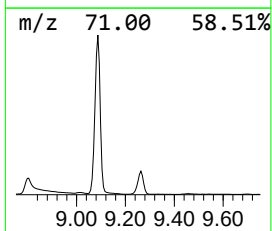
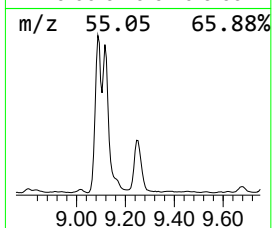
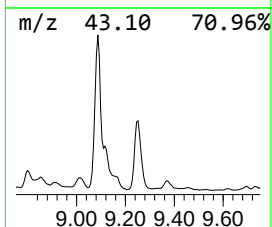
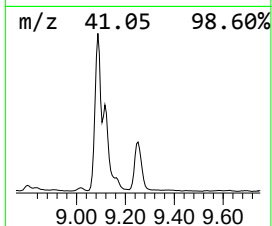
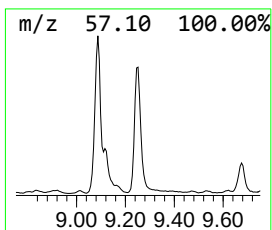
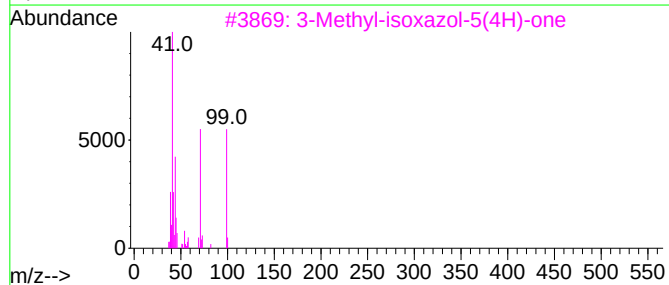
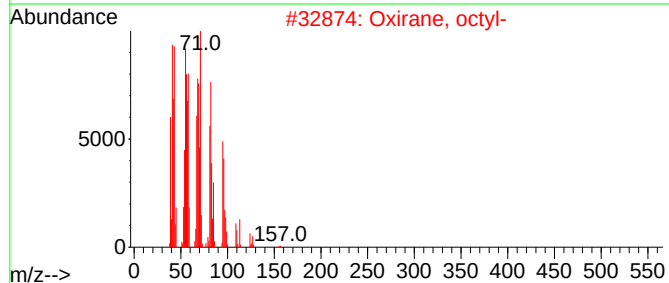
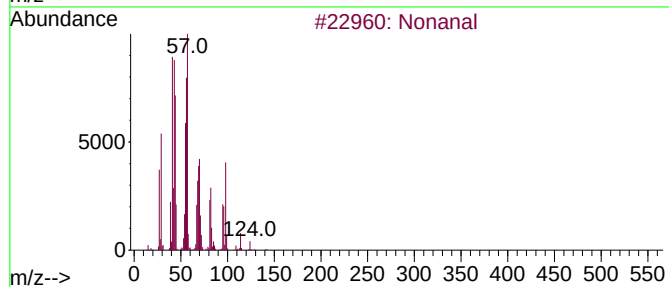
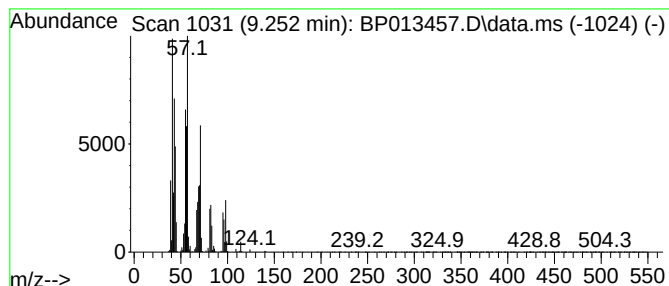
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.252	48.99 ng	6650140	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	72
2			Oxirane, octyl-	156	C10H20O	002404-44-6	38
3			3-Methyl-isoxazol-5(4H)-one	99	C4H5N02	001517-96-0	22
4			3-Methyl-5-hydroxy-isoxazole	99	C4H5N02	045469-93-0	22
5			Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-14-02

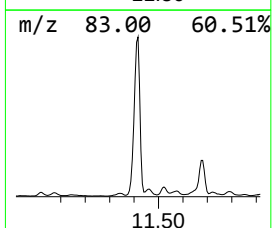
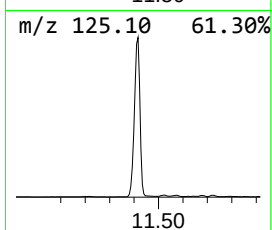
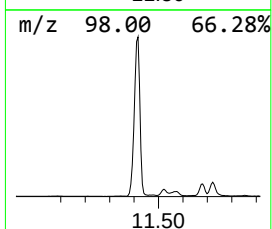
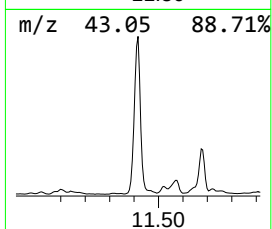
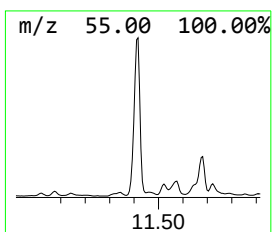
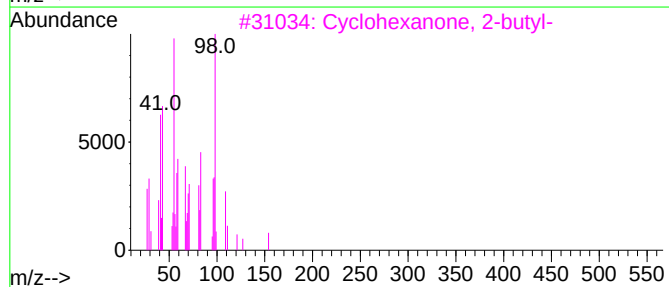
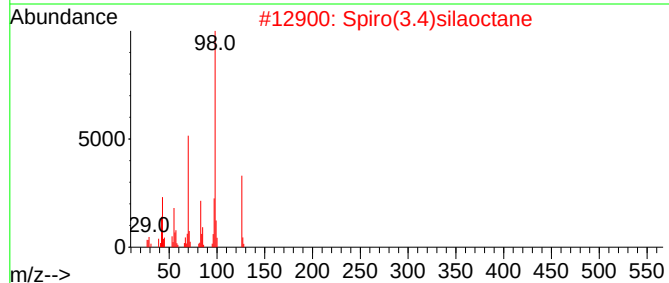
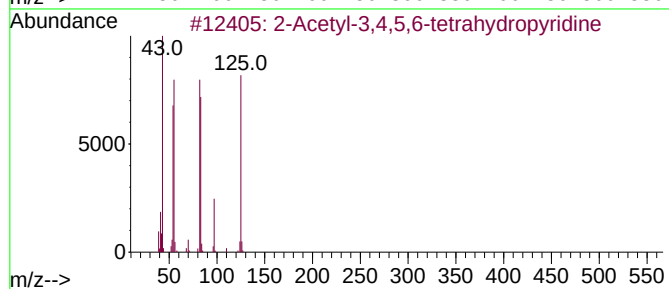
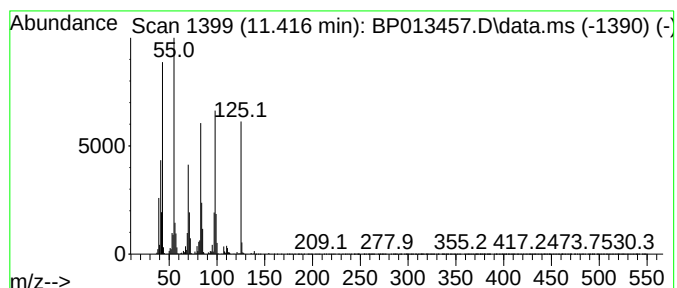
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown11.416 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.416	95.17 ng	21535100	Naphthalene-d8	10.740

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Acetyl-3,4,5,6-tetrahydropyridine	125	C7H11NO	027300-27-2	38	
2	Spiro(3.4)silaoctane	126	C7H14Si	1000433-94-6	38	
3	Cyclohexanone, 2-butyl-	154	C10H18O	001126-18-7	38	
4	Cycloheptane	98	C7H14	000291-64-5	35	
5	1-Nonene	126	C9H18	000124-11-8	35	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
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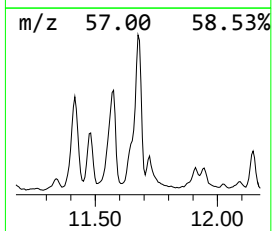
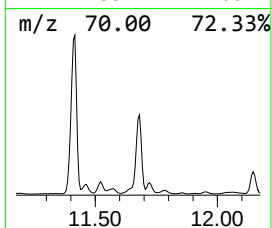
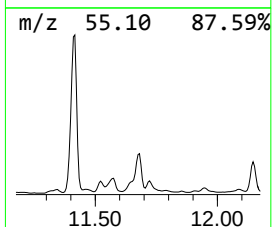
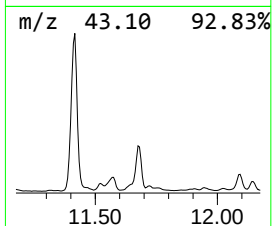
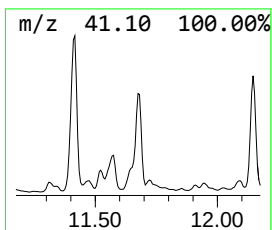
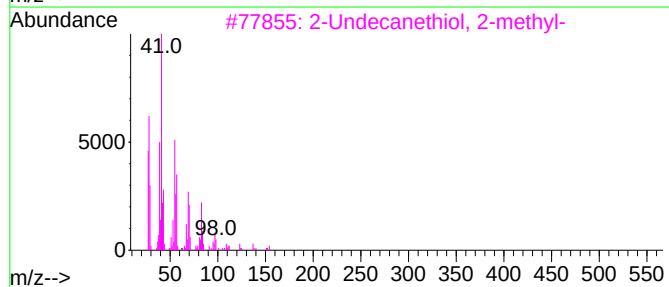
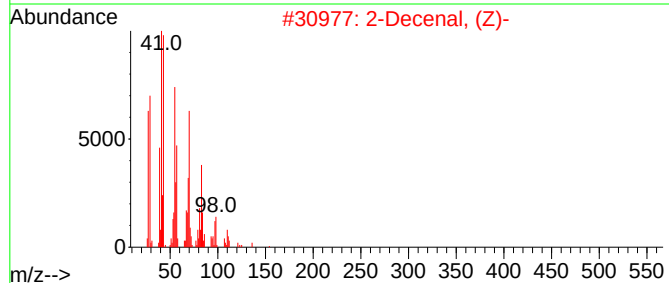
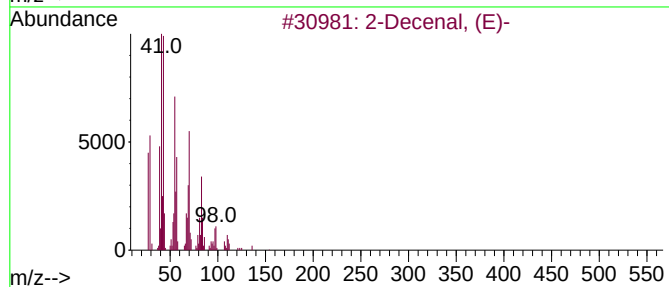
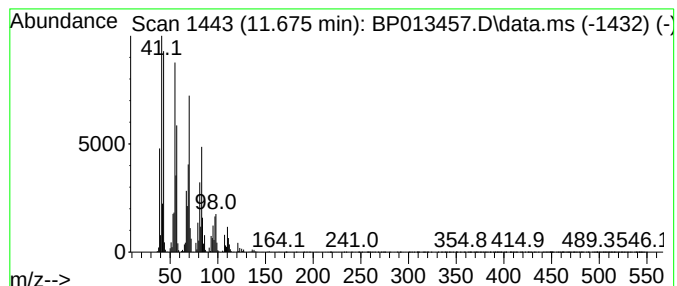
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Decenal, (E)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.675	41.23 ng	9328630	Naphthalene-d8	10.740	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decenal, (E)-	154	C10H18O	003913-81-3	64
2	2-Decenal, (Z)-	154	C10H18O	002497-25-8	62
3	2-Undecanethiol, 2-methyl-	202	C12H26S	010059-13-9	53
4	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	49
5	2-Heptenal, (E)-	112	C7H12O	018829-55-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
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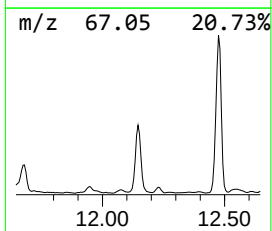
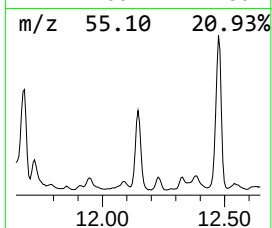
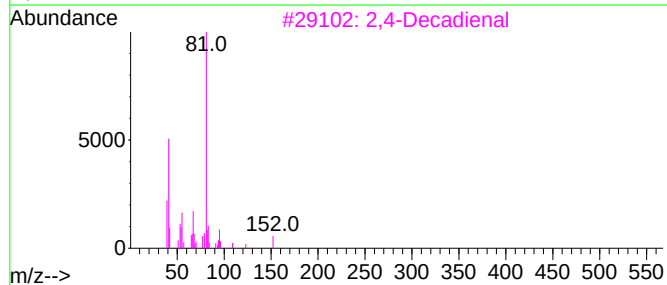
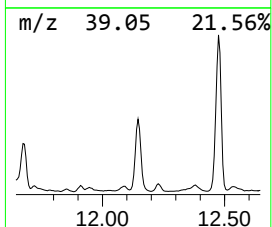
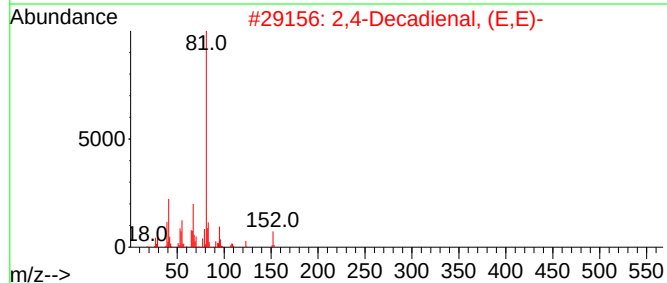
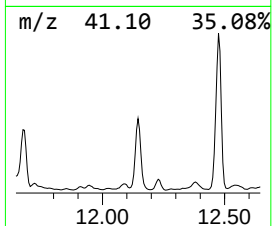
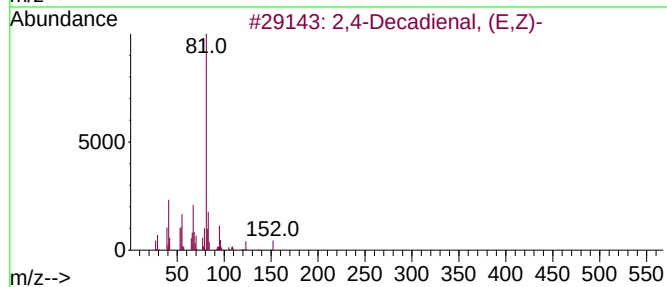
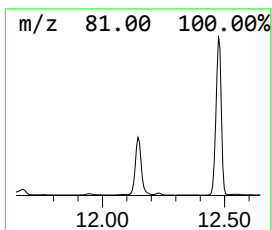
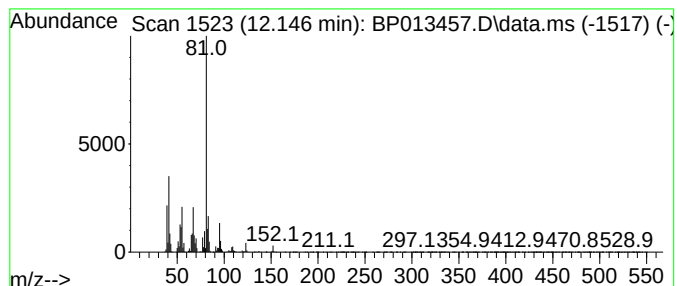
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ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2,4-Decadienal, (E,Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.146	43.03 ng	9736140	Naphthalene-d8	10.740	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Decadienal, (E,Z)-	152	C10H16O	025152-83-4	97
2	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	91
3	2,4-Decadienal	152	C10H16O	002363-88-4	90
4	2,4-Nonadienal	138	C9H14O	006750-03-4	86
5	2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
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Operator : CG/JU
Sample : 01064-07 10X
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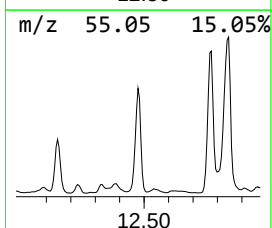
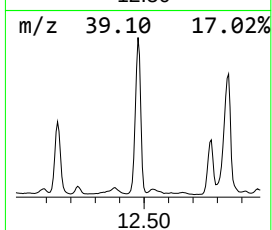
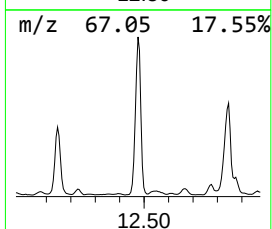
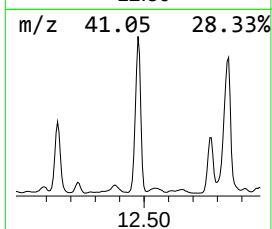
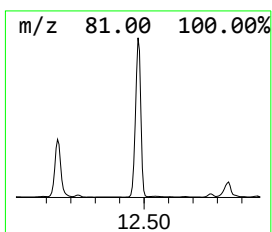
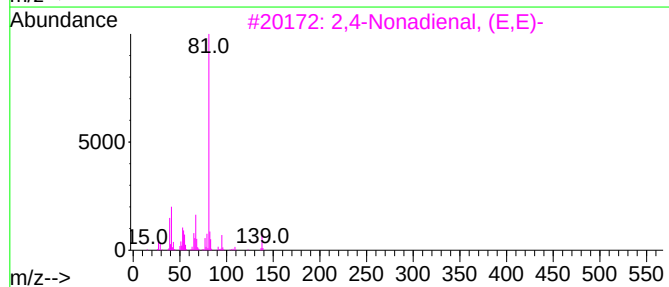
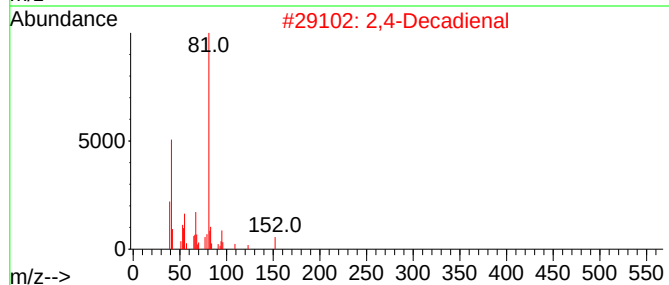
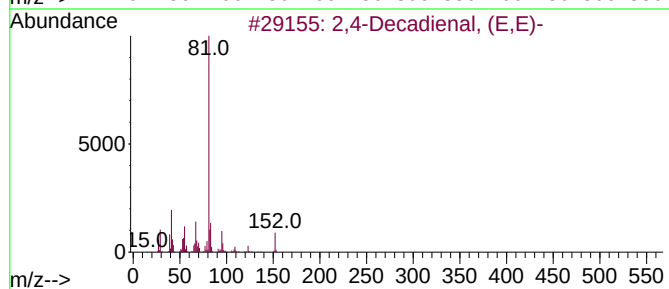
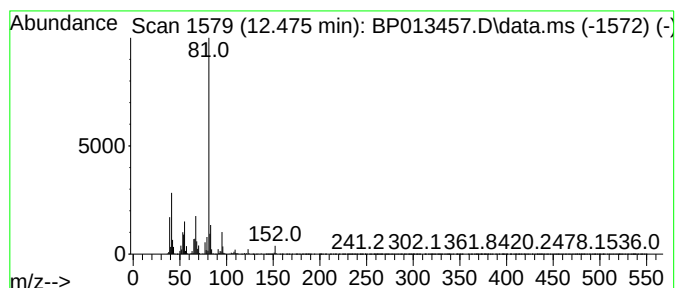
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2,4-Decadienal, (E,E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.475	91.35 ng	20672000	Naphthalene-d8	10.740	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	93
2	2,4-Decadienal	152	C10H16O	002363-88-4	91
3	2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	78
4	2,4-Nonadienal	138	C9H14O	006750-03-4	78
5	2,4-Octadienal, (E,E)-	124	C8H12O	030361-28-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-14-02

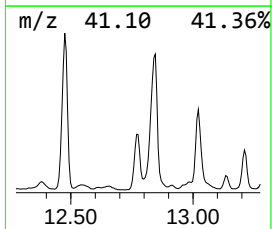
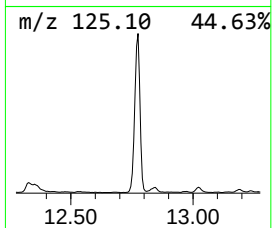
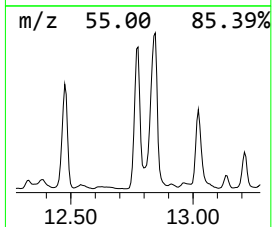
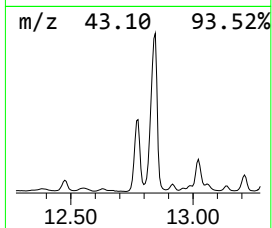
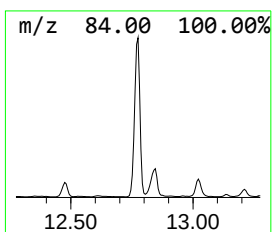
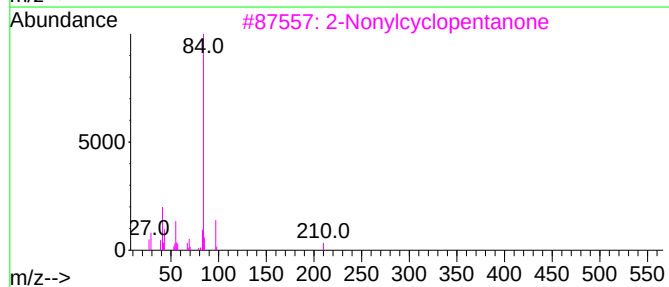
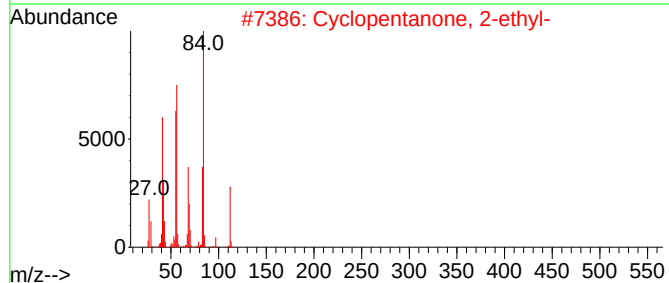
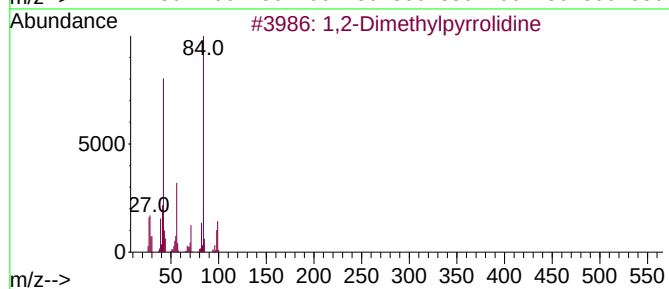
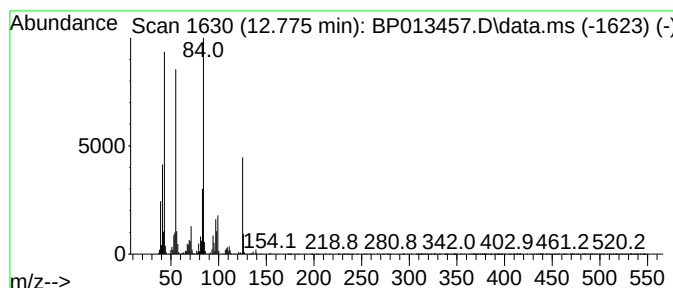
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown12.775 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.775	32.31 ng	10712300	Acenaphthene-d10	14.569

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Dimethylpyrrolidine	99	C6H13N	1000326-00-9	38
2		Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	38
3		2-Nonylcyclopentanone	210	C14H26O	1000433-19-9	38
4		2-Methylpiperidine	99	C6H13N	000109-05-7	38
5		2-Butylcyclopentanone	140	C9H16O	1000433-20-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

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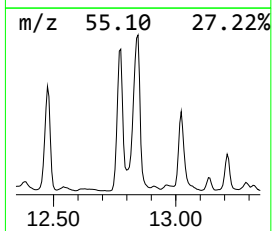
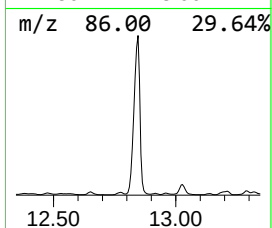
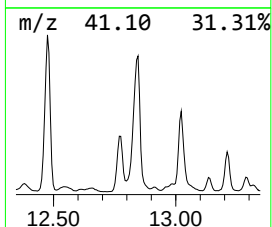
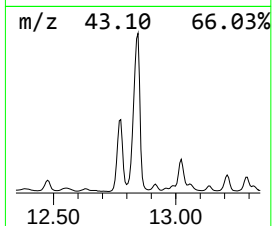
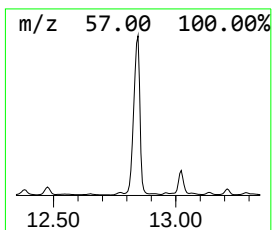
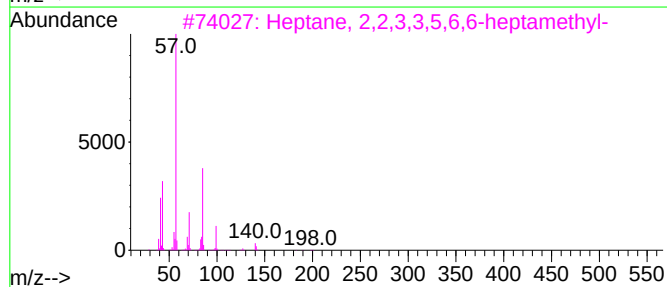
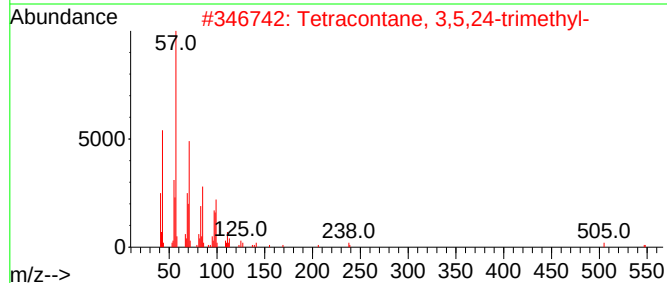
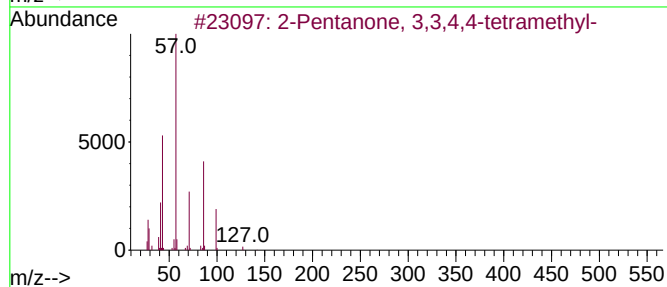
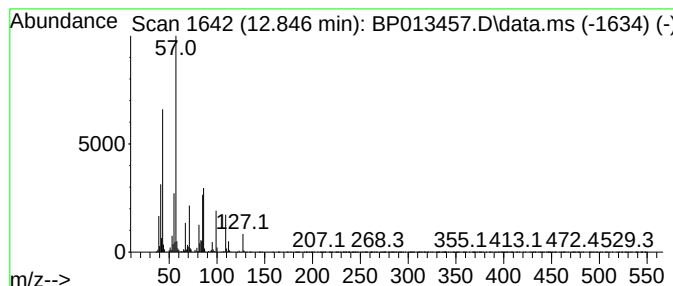
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown12.846 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.846	88.51 ng	29343200	Acenaphthene-d10	14.569

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 3,3,4,4-tetramethyl-	142	C9H18O	000865-66-7	38
2		Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	38
3		Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	38
4		Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	38
5		Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

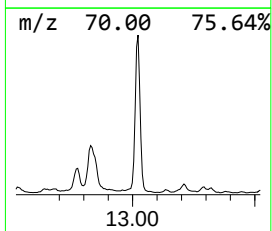
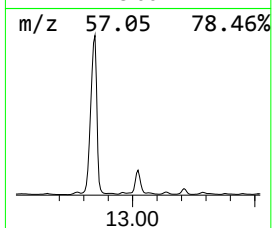
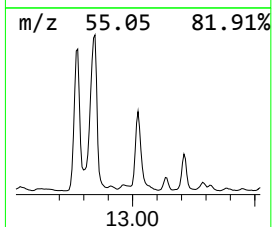
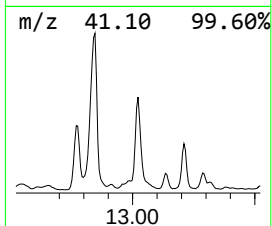
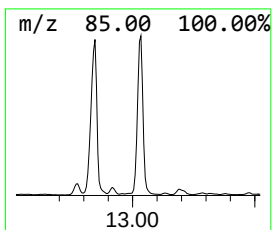
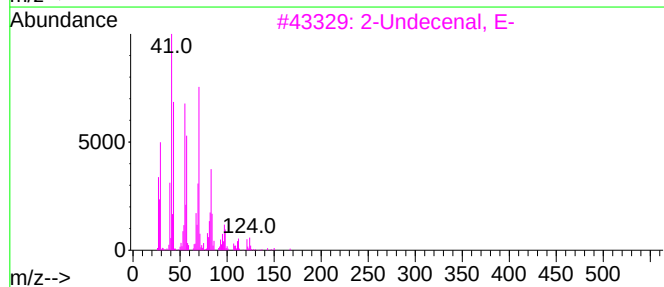
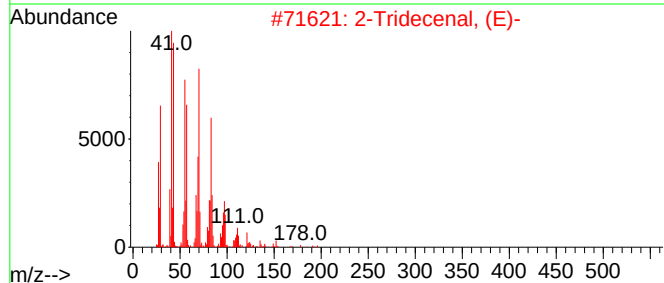
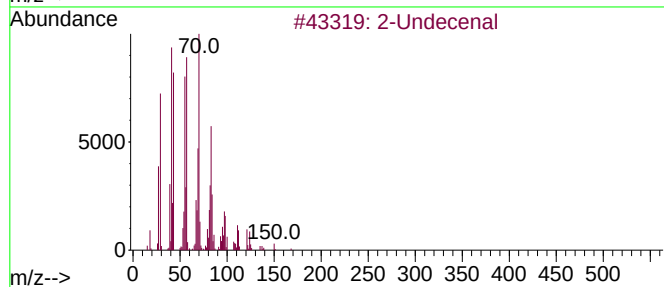
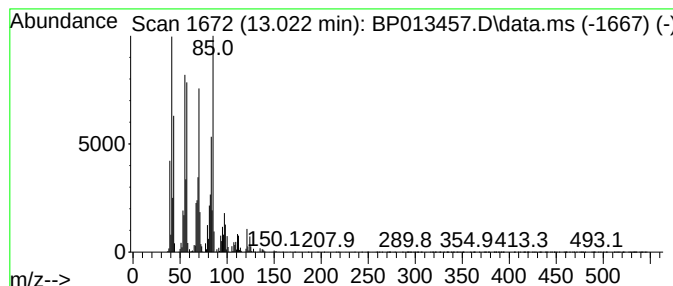
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2-Undecenal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.022	34.92 ng	11575100	Acenaphthene-d10		14.569	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Undecenal		168	C11H20O	002463-77-6	58
2	2-Tridecenal, (E)-		196	C13H24O	007069-41-2	52
3	2-Undecenal, E-		168	C11H20O	053448-07-0	49
4	2-Decenal, (E)-		154	C10H18O	003913-81-3	47
5	2-Methylene cyclopentanol		98	C6H10O	020461-31-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

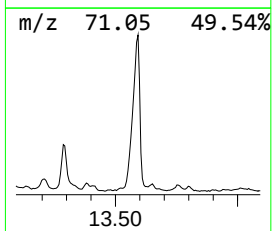
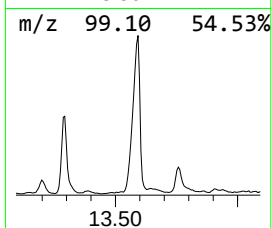
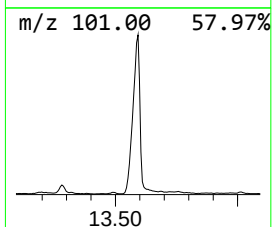
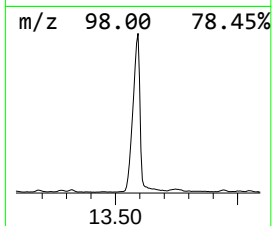
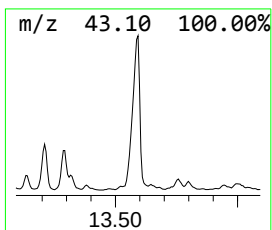
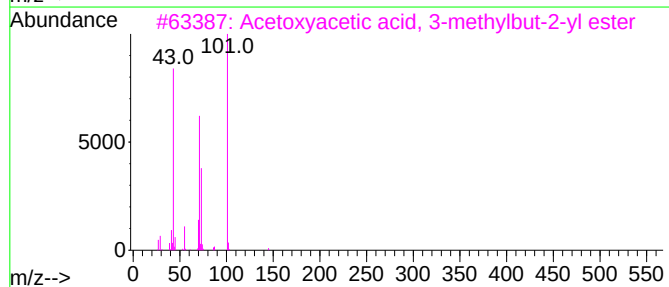
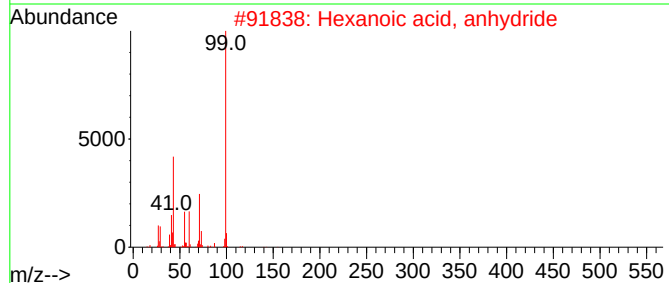
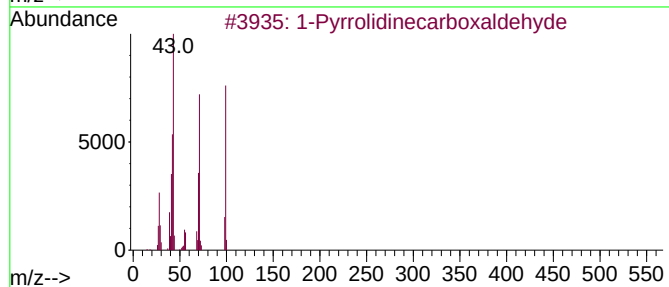
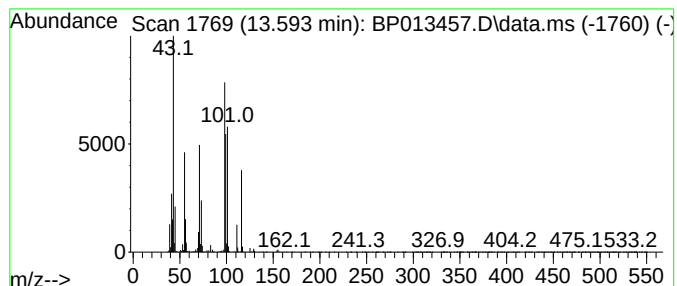
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown13.593 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.593	25.64 ng	8499510	Acenaphthene-d10		14.569	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Pyrrolidinecarboxaldehyde		99	C5H9NO	003760-54-1	22
2	Hexanoic acid, anhydride		214	C12H22O3	002051-49-2	22
3	Acetoxyacetic acid, 3-methylbut-...		188	C9H16O4	1000355-69-8	16
4	Pentanoic acid, 2-methyl-, anhyd...		214	C12H22O3	063169-61-9	14
5	3-Isoxazoline, 5-methyl-		98	C4H6N2O	001072-67-9	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

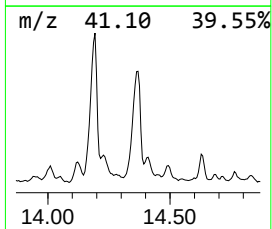
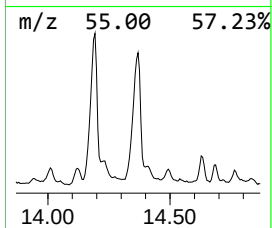
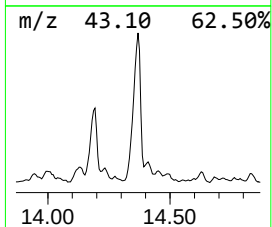
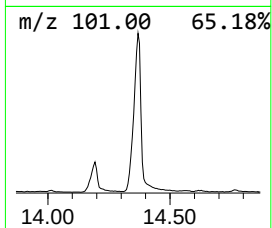
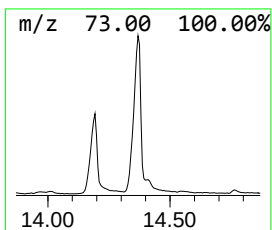
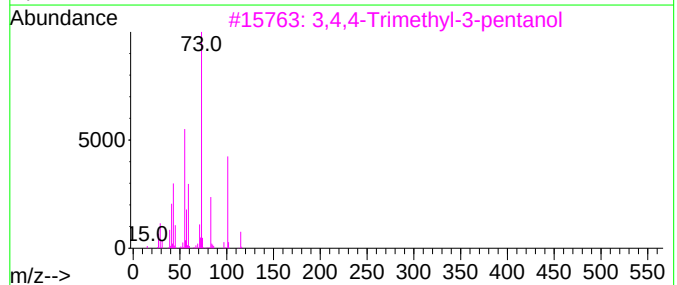
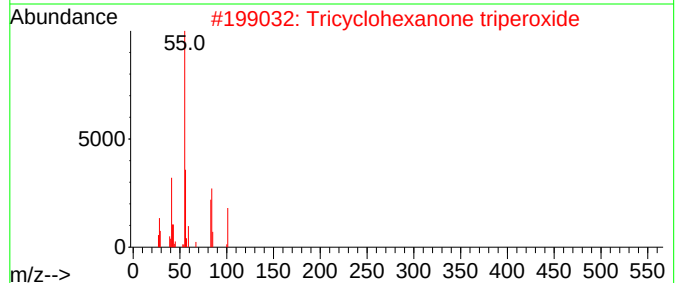
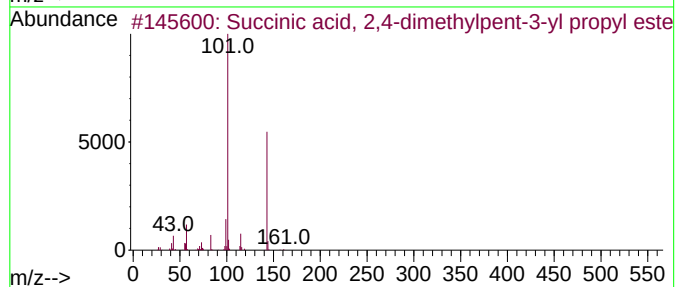
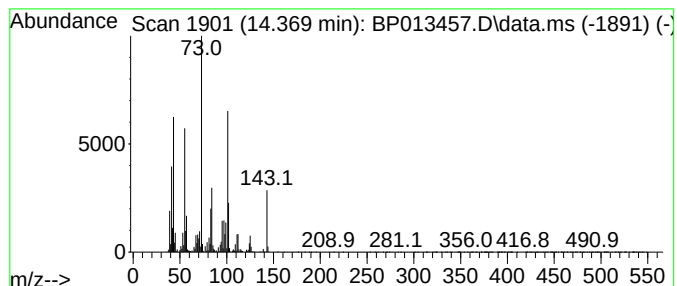
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S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown14.369 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.369	28.50 ng	9447320	Acenaphthene-d10		14.569
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 2,4-dimethylpent-...	258	C14H26O4	1010349-25-6	32
2	Tricyclohexanone triperoxide	300	C15H24O6	1000357-14-9	25
3	3,4,4-Trimethyl-3-pentanol	130	C8H18O	007294-05-5	12
4	Succinic acid, tridec-2-yn-1-yl ...	380	C23H40O4	1000389-62-1	12
5	1,3-Dioxolane, 4,5-dimethyl-2-pe...	312	C20H40O2	056599-61-2	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

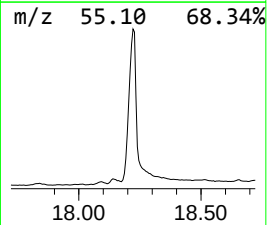
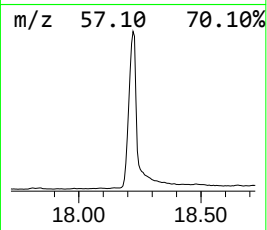
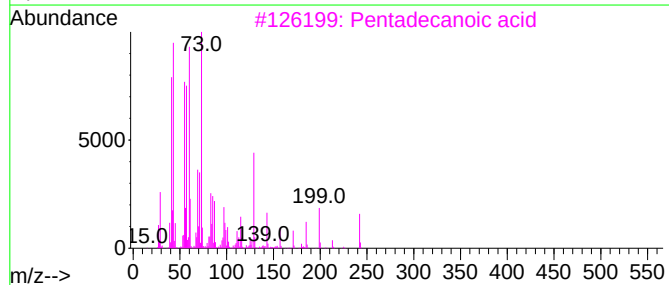
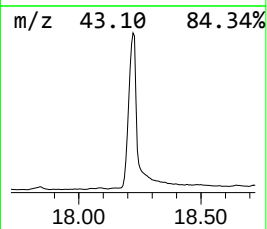
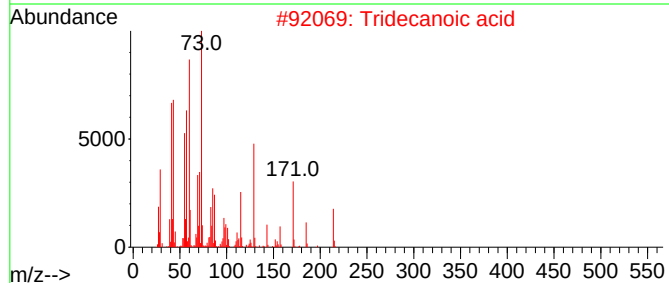
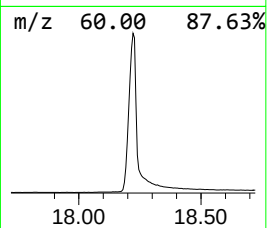
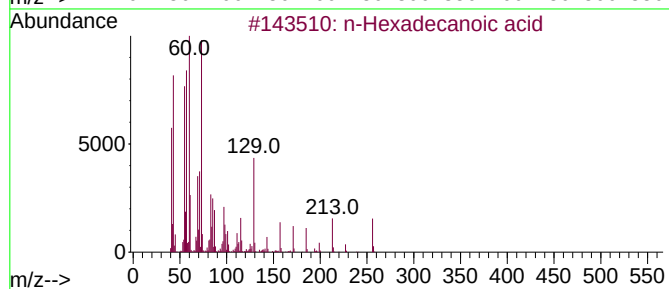
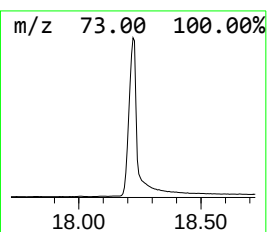
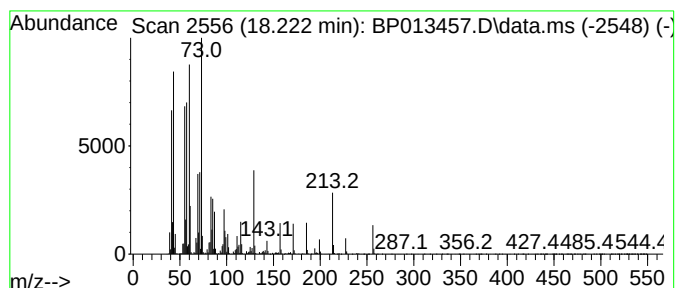
Instrument :
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ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.222	123.46 ng	61620000	Phenanthrene-d10		17.328	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
5	n-Decanoic acid		172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

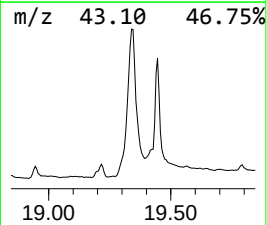
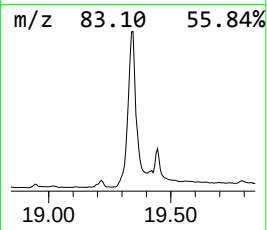
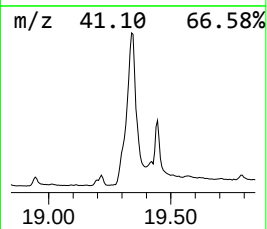
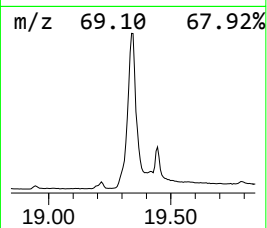
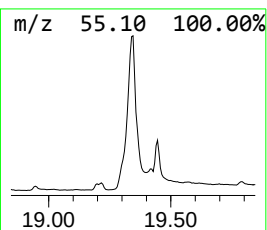
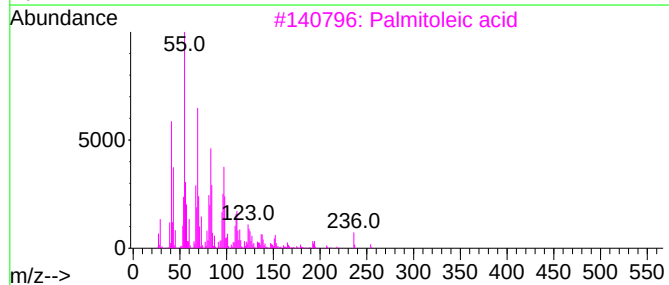
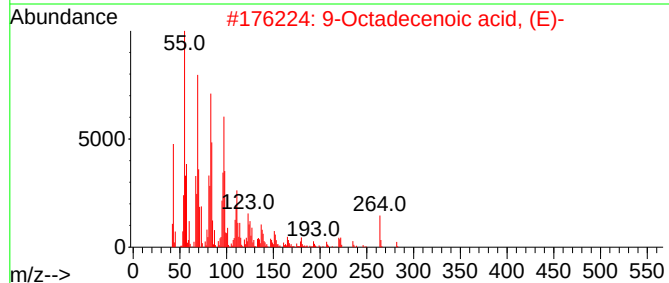
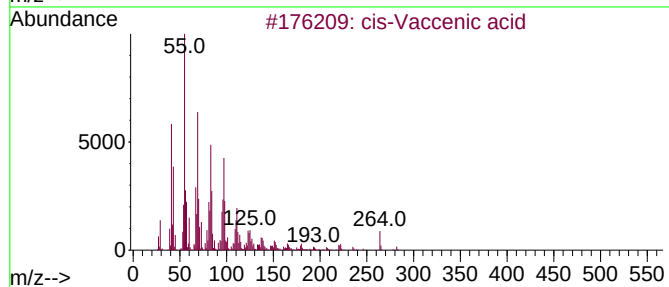
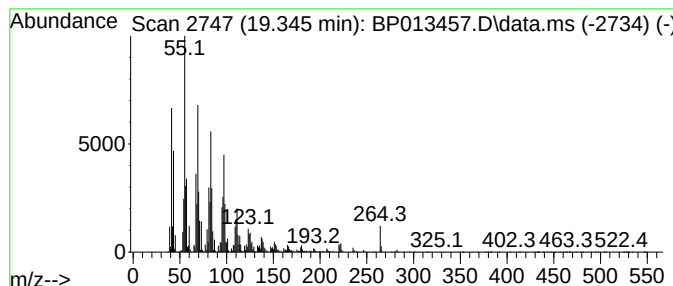
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ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 cis-Vaccenic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.345	157.61 ng	78663500	Phenanthrene-d10		17.328	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid		282	C18H34O2	000506-17-2	94
2	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	93
3	Palmitoleic acid		254	C16H30O2	000373-49-9	93
4	cis-13-Octadecenoic acid		282	C18H34O2	013126-39-1	91
5	6-Octadecenoic acid, (Z)-		282	C18H34O2	000593-39-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

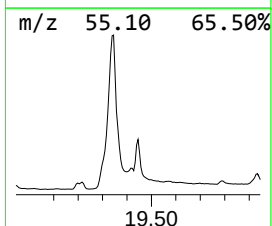
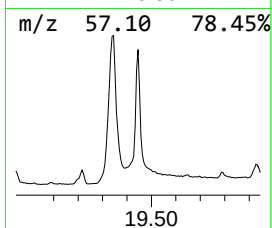
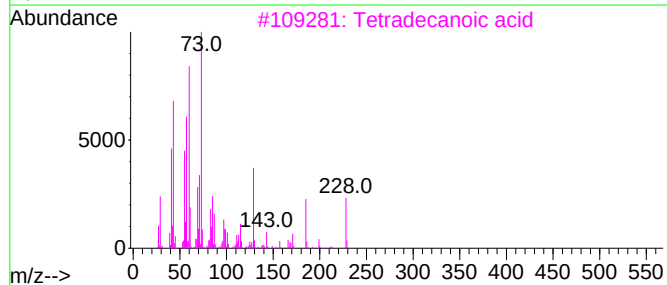
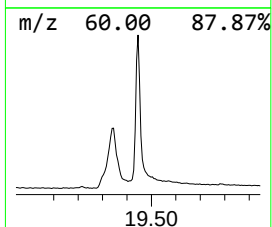
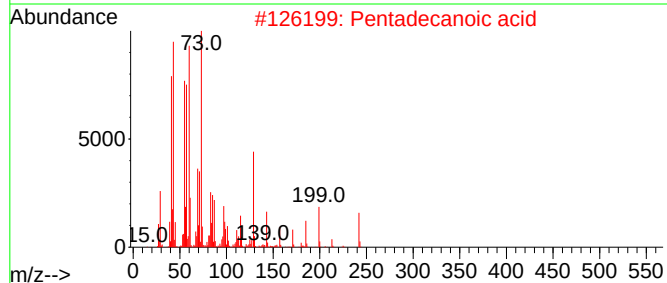
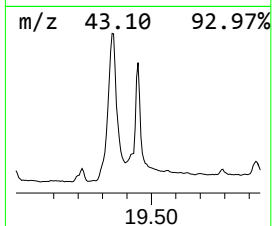
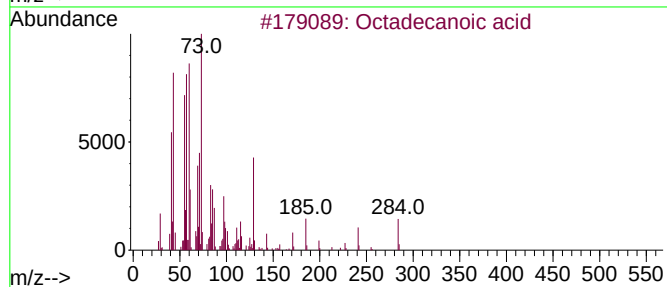
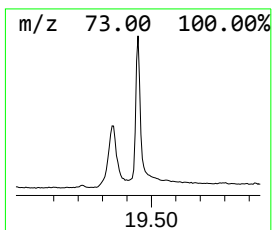
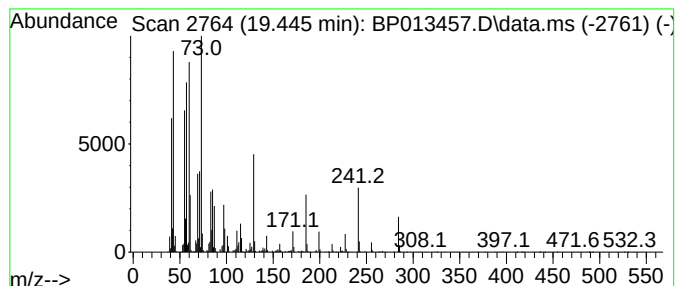
Instrument :
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ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.445	35.80 ng	16648200	Chrysene-d12	21.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013457.D
Acq On : 11 Jan 2023 22:45
Operator : CG/JU
Sample : 01064-07 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-14-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.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
Butanal, 3-methyl-	3.223	42.4	ng	5752760	1	7.922	2714920	20.0
Hexanal	4.446	504.1	ng	68435300	1	7.922	2714920	20.0
1-Hexanol	5.399	43.3	ng	5881630	1	7.922	2714920	20.0
2-Heptenal, (E)-	6.869	32.6	ng	4426290	1	7.922	2714920	20.0
Hexanoic acid	7.022	35.5	ng	4813420	1	7.922	2714920	20.0
Furan, 2-pentyl-	7.405	30.7	ng	4165040	1	7.922	2714920	20.0
Acetic caproic ...	8.540	93.8	ng	12725600	1	7.922	2714920	20.0
Nonanal	9.252	49.0	ng	6650140	1	7.922	2714920	20.0
unknown11.416	11.416	95.2	ng	21535100	2	10.740	4525710	20.0
2-Decenal, (E)-	11.675	41.2	ng	9328630	2	10.740	4525710	20.0
2,4-Decadienal,...	12.146	43.0	ng	9736140	2	10.740	4525710	20.0
2,4-Decadienal,...	12.475	91.3	ng	20672000	2	10.740	4525710	20.0
unknown12.775	12.775	32.3	ng	10712300	3	14.569	6630320	20.0
unknown12.846	12.846	88.5	ng	29343200	3	14.569	6630320	20.0
2-Undecenal	13.022	34.9	ng	11575100	3	14.569	6630320	20.0
unknown13.593	13.593	25.6	ng	8499510	3	14.569	6630320	20.0
unknown14.369	14.369	28.5	ng	9447320	3	14.569	6630320	20.0
n-Hexadecanoic ...	18.222	123.5	ng	61620000	4	17.328	9981850	20.0
cis-Vaccenic acid	19.345	157.6	ng	78663500	4	17.328	9981850	20.0
Octadecanoic acid	19.445	35.8	ng	16648200	5	21.416	9300050	20.0