

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
 Data File : BF127693.D
 Acq On : 07 Apr 2022 19:59
 Operator : CG\JU
 Sample : N2270-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FARMINGDALE-CLAY-1

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_F\Methods\8270-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127693.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.310	3	4	10	rVB	293589	260915	5.27%	0.892%
2	3.187	147	153	162	rVB	32199	53128	1.07%	0.182%
3	5.204	488	496	501	rBV	51653	66655	1.35%	0.228%
4	5.581	555	560	563	rBV	2755016	2635536	53.20%	9.007%
5	6.575	723	729	732	rBV	2590421	2767786	55.87%	9.459%
6	6.963	791	795	798	rBV	909465	715837	14.45%	2.446%
7	7.522	885	890	894	rBV	1718587	1818826	36.71%	6.216%
8	8.139	992	995	1003	rBV	114040	114578	2.31%	0.392%
9	8.245	1009	1013	1016	rBV	1128305	928497	18.74%	3.173%
10	9.322	1191	1196	1200	rBV	3429378	3361431	67.85%	11.488%
11	10.004	1308	1312	1316	rBV	1181530	1107509	22.35%	3.785%
12	10.798	1440	1447	1450	rBV	2551868	2244173	45.30%	7.669%
13	10.892	1459	1463	1466	rBV	1134058	920747	18.58%	3.147%
14	11.351	1538	1541	1544	rBV	43790	49880	1.01%	0.170%
15	11.498	1562	1566	1569	rBV	1353977	1173426	23.68%	4.010%
16	12.716	1770	1773	1781	rVB	49784	60005	1.21%	0.205%
17	13.039	1824	1828	1831	rBV	64339	56791	1.15%	0.194%
18	13.092	1832	1837	1840	rBV	3899220	3466398	69.97%	11.846%
19	13.986	1985	1989	2005	rBV	260036	476074	9.61%	1.627%
20	14.145	2010	2016	2020	rBV	965011	934446	18.86%	3.193%
21	14.568	2070	2088	2106	rBV2	1122126	4954336	100.00%	16.931%
22	14.857	2128	2137	2147	rVB7	41103	160065	3.23%	0.547%
23	15.674	2270	2276	2286	rVB	651977	827814	16.71%	2.829%
24	16.027	2328	2336	2349	rVB	31076	106564	2.15%	0.364%

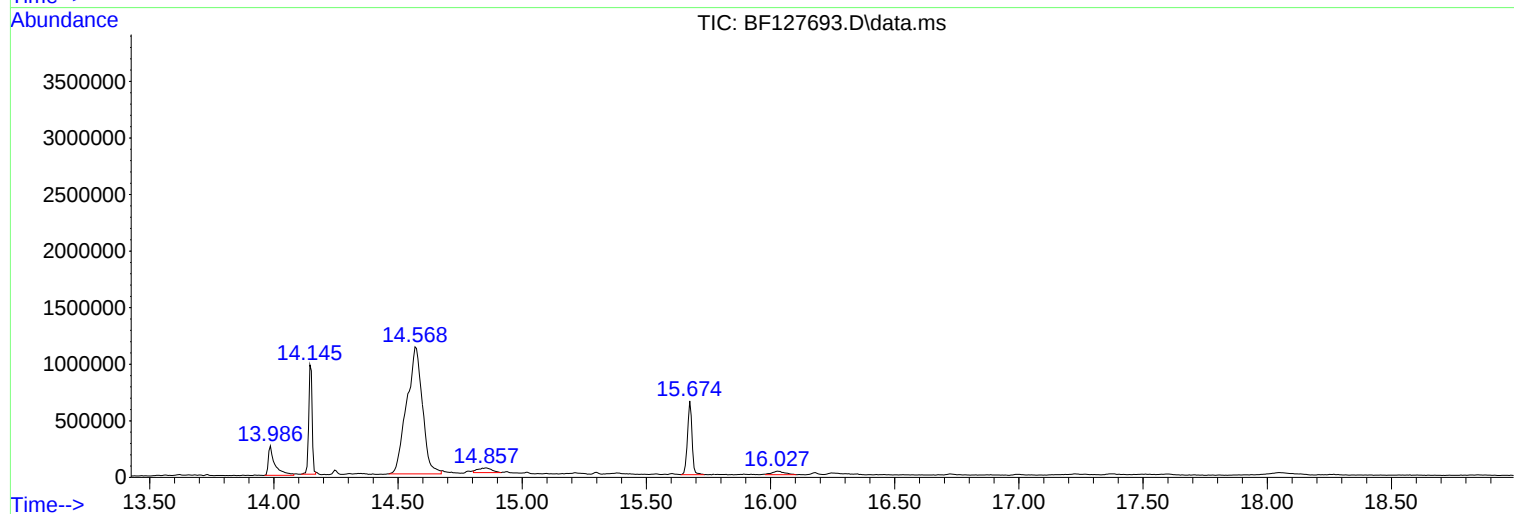
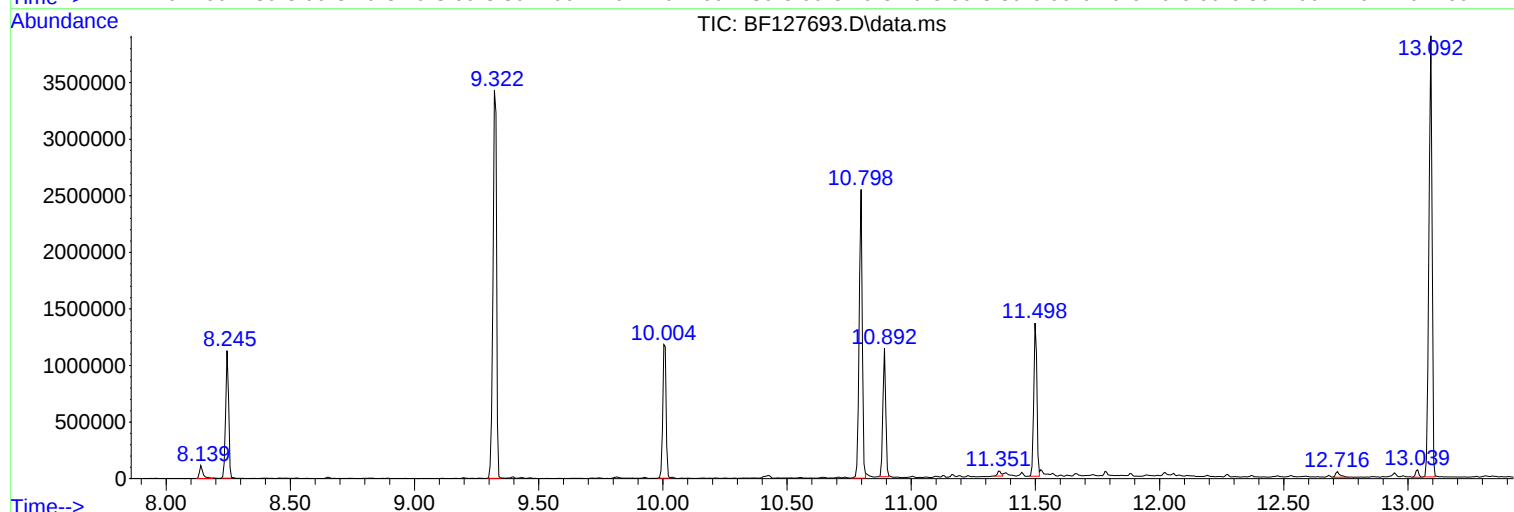
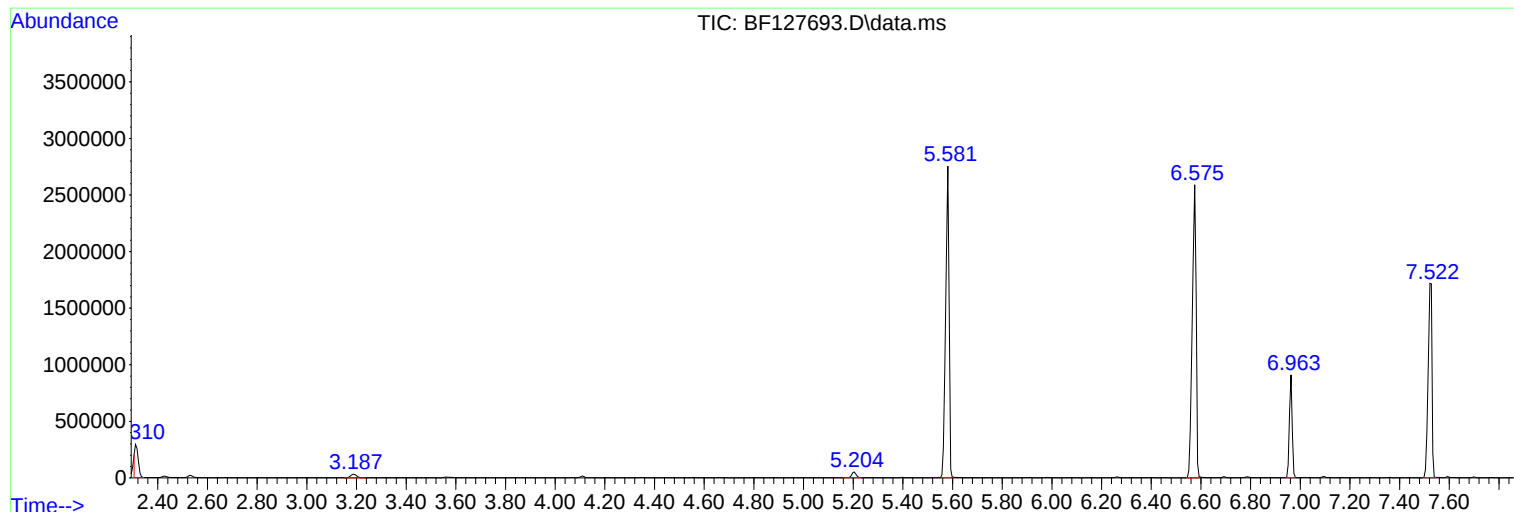
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Instrument :
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ClientSampleId :
FARMINGDALE-CLAY-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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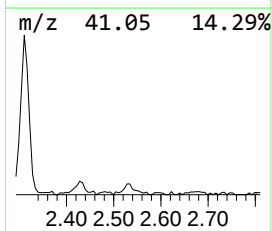
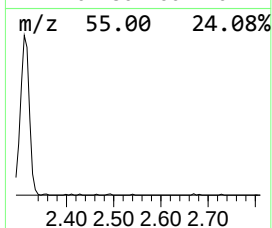
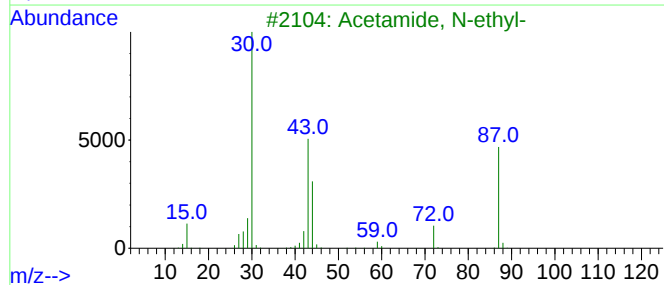
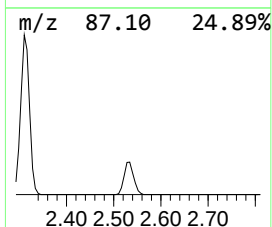
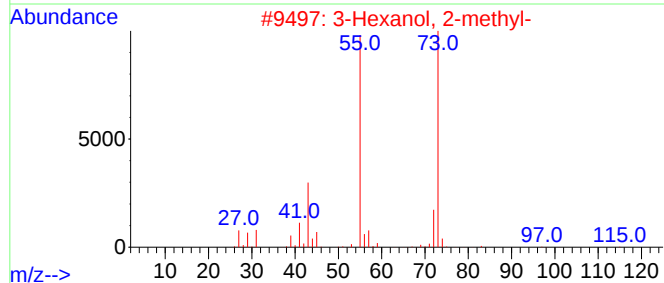
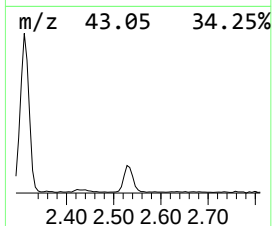
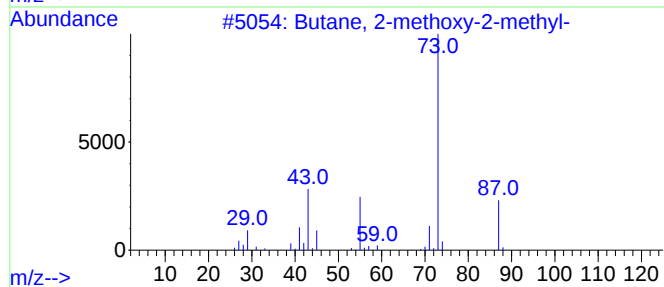
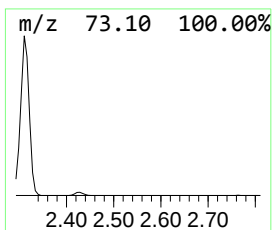
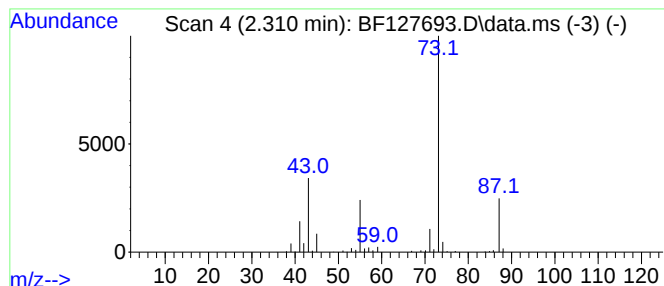
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.310	7.29 ng	260915	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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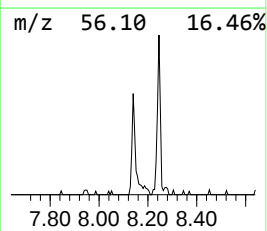
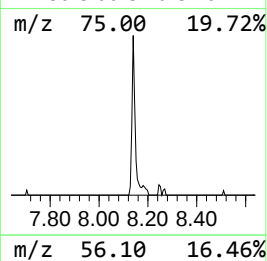
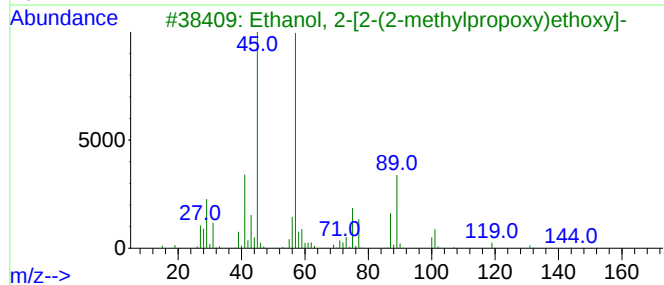
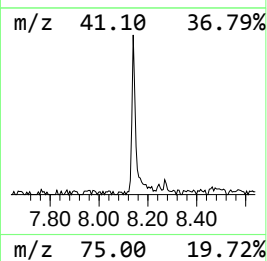
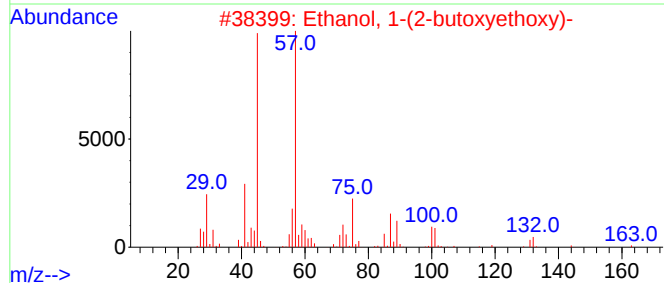
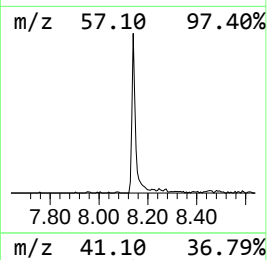
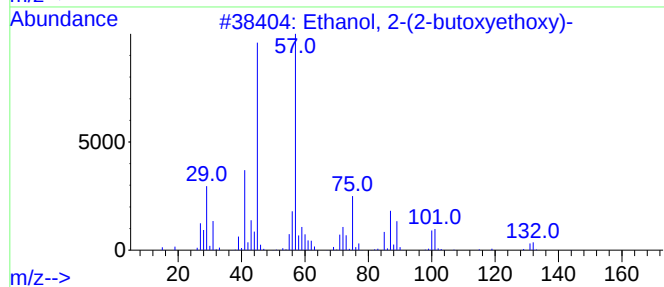
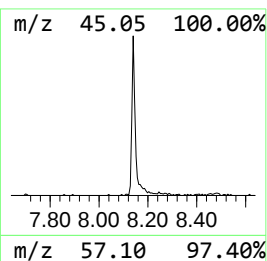
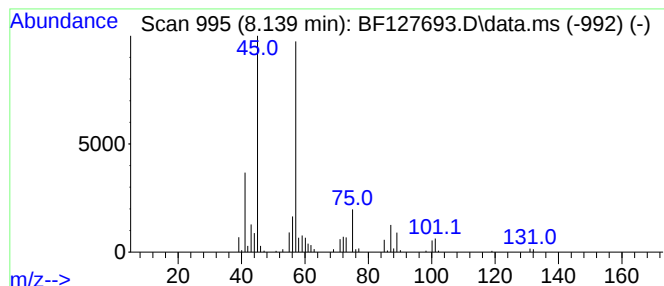
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.139	2.47 ng	114578	Naphthalene-d8	8.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47



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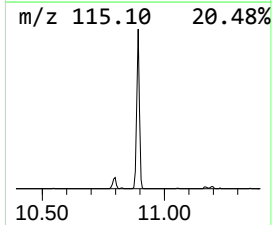
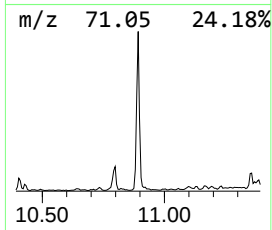
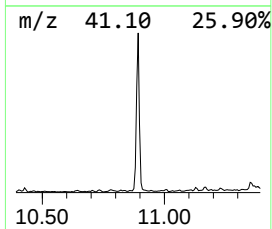
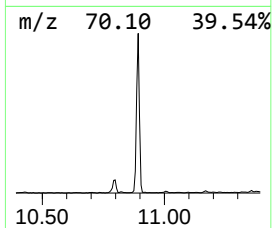
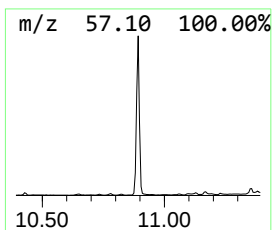
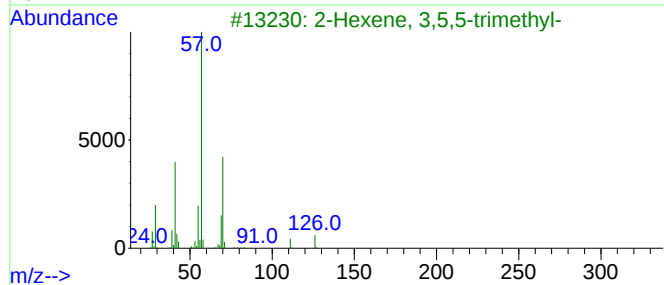
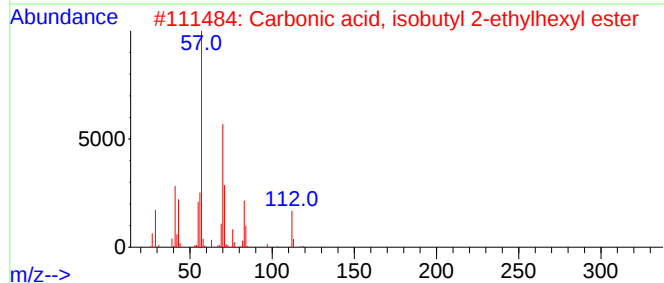
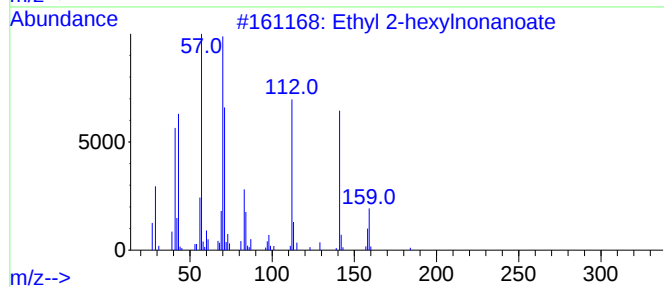
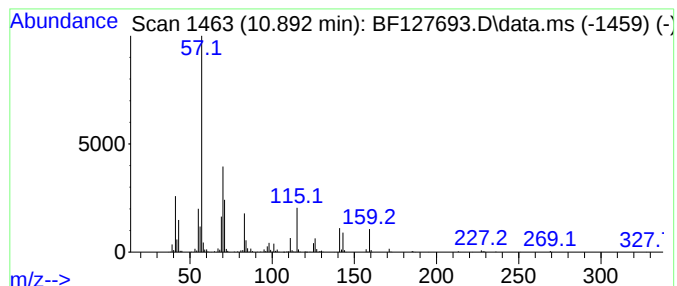
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.892 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.892	15.69 ng	920747	Phenanthrene-d10	11.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl 2-hexylnonanoate	270	C17H34O2	1000433-21-8	47
2			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	43
3			2-Hexene, 3,5,5-trimethyl-	126	C9H18	026456-76-8	43
4			3,5,5-Trimethylhexyl propionate	200	C12H24O2	1000429-26-0	38
5			2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	37



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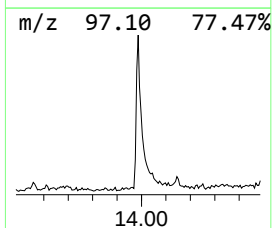
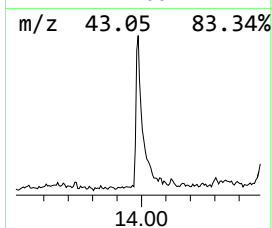
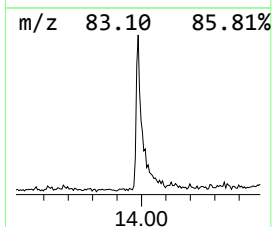
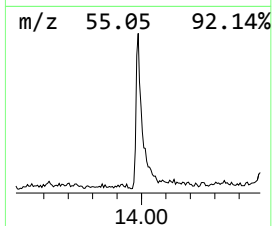
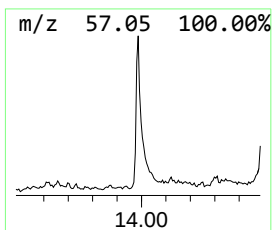
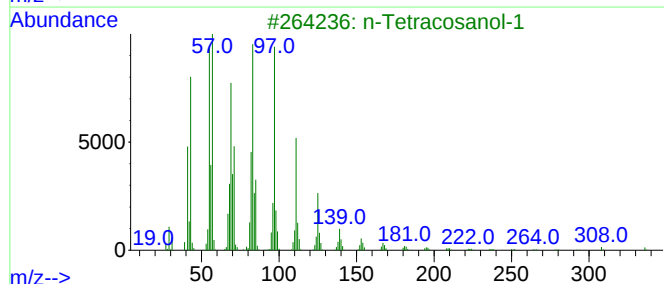
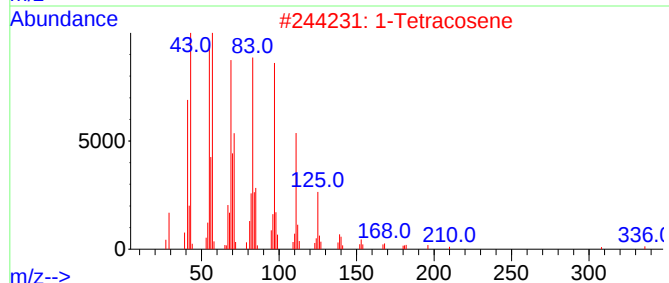
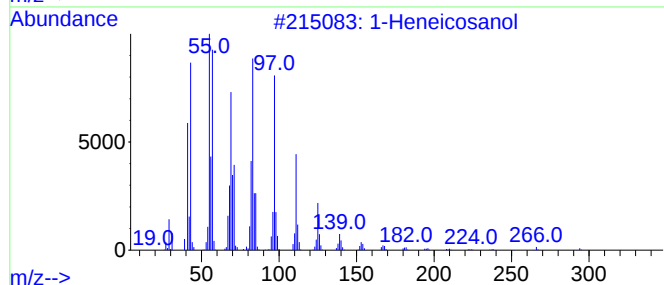
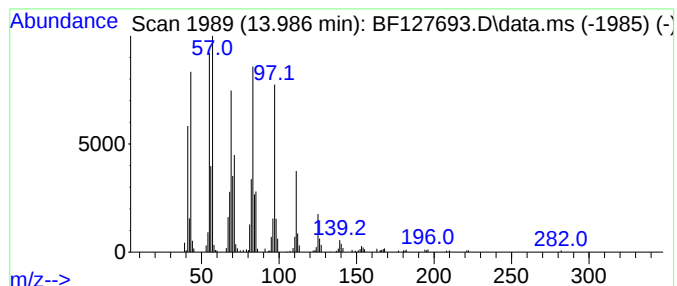
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	10.19 ng	476074	Chrysene-d12	14.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Tetracosene	336	C24H48	010192-32-2	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Behenic alcohol	326	C22H46O	000661-19-8	94



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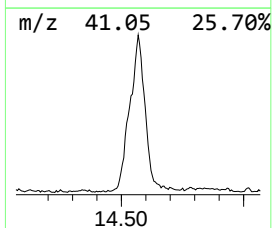
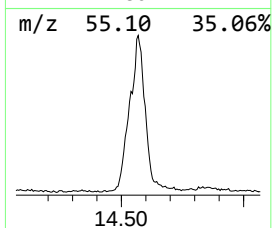
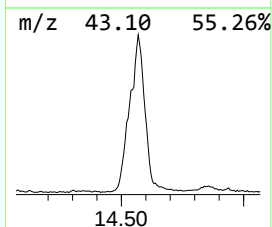
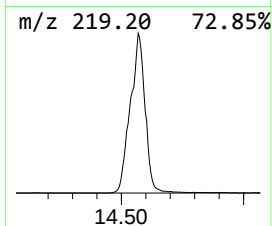
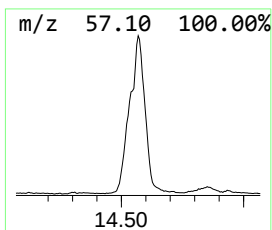
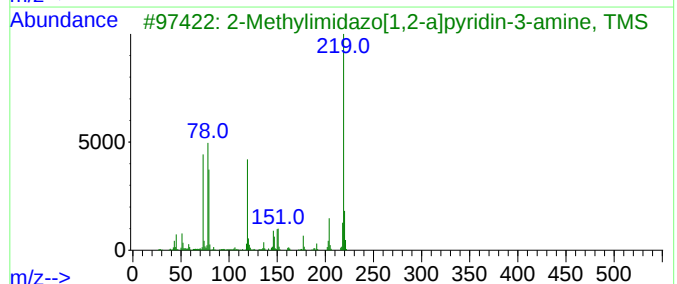
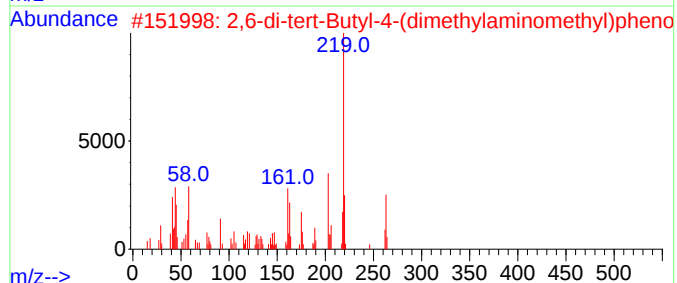
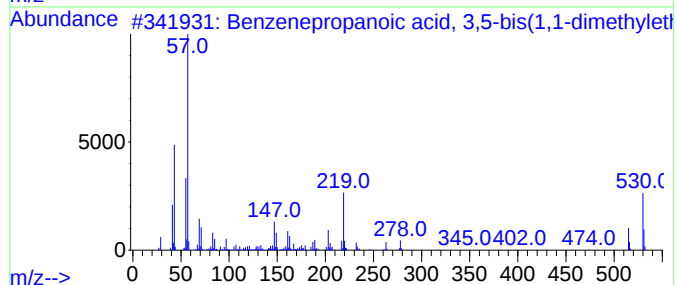
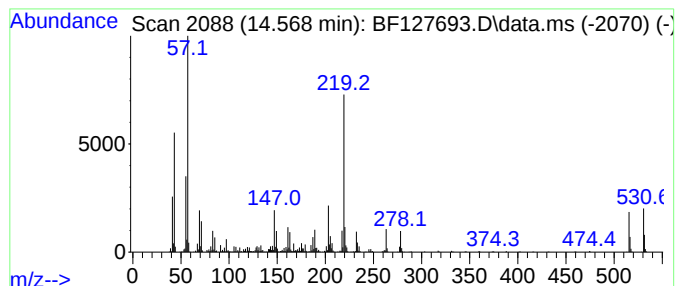
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Peak Number 5 Benzenepropanoic acid, 3,5-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.569	106.04 ng	4954340	Chrysene-d12	14.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanoic acid, 3,5-bis(1...	530	C35H62O3	002082-79-3	99
2			2,6-di-tert-Butyl-4-(dimethylami...	263	C17H29NO	000088-27-7	30
3			2-Methylimidazo[1,2-a]pyridin-3-...	219	C11H17N3Si	1000508-69-8	30
4			acetamide, 2,2,2-trifluoro-N-(4-...	219	C9H8F3NO2	1010400-75-8	25
5			Quinoline, 3-(4-methylphenyl)-	219	C16H13N	1000380-55-4	25



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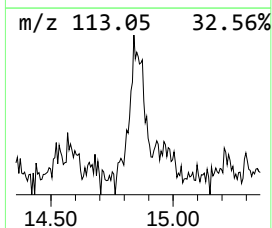
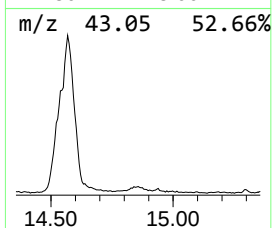
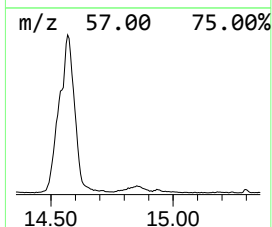
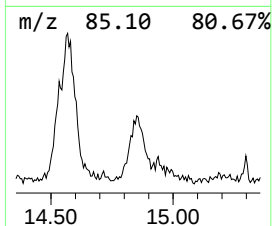
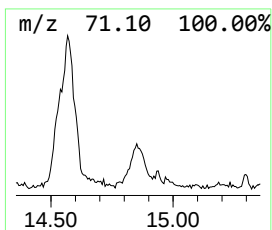
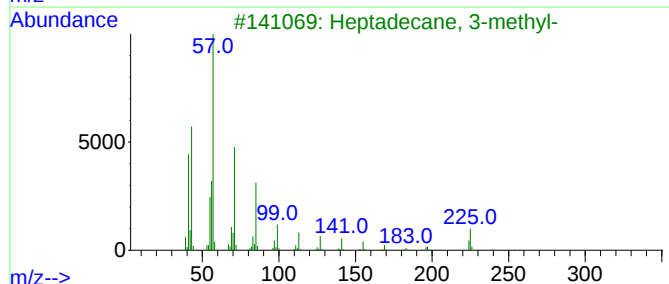
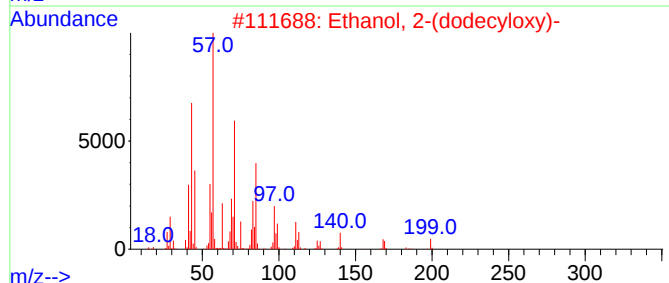
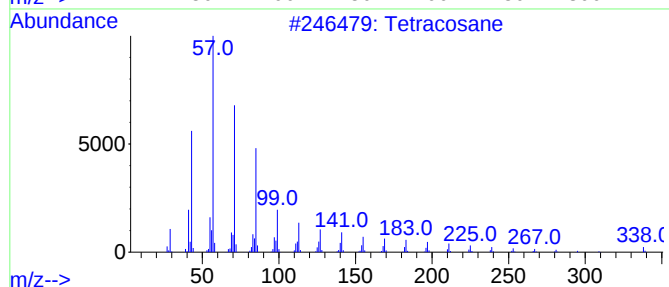
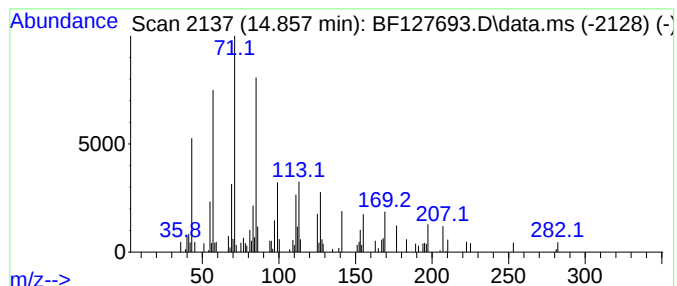
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	3.43 ng	160065	Chrysene-d12	14.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	72
2			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	64
3			Heptadecane, 3-methyl-	254	C18H38	006418-44-6	64
4			Eicosane	282	C20H42	000112-95-8	64
5			Octacosane	394	C28H58	000630-02-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127693.D
Acq On : 07 Apr 2022 19:59
Operator : CG\JU
Sample : N2270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FARMINGDALE-CLAY-1

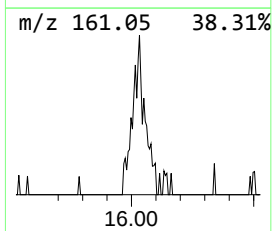
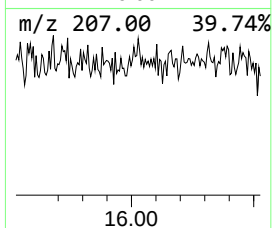
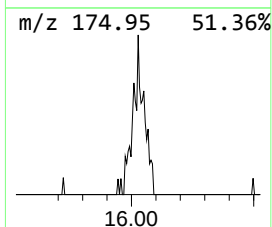
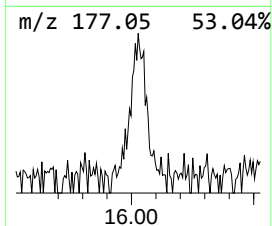
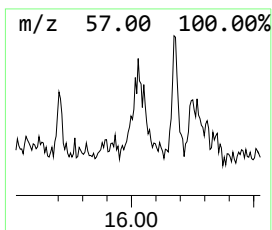
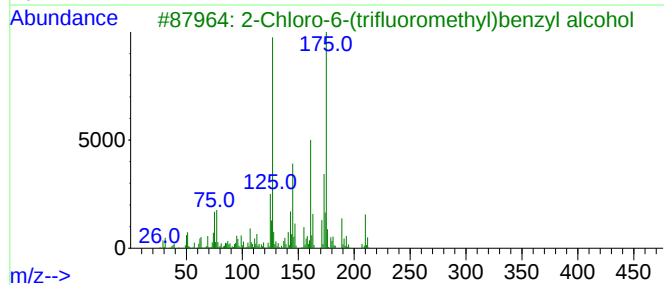
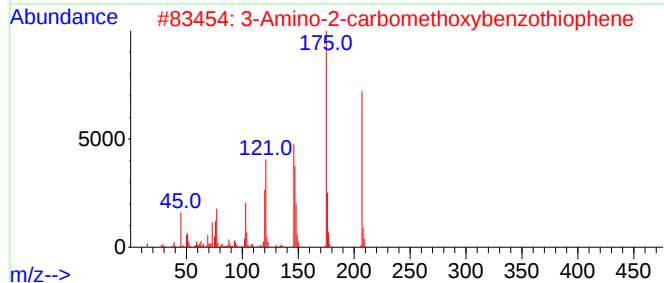
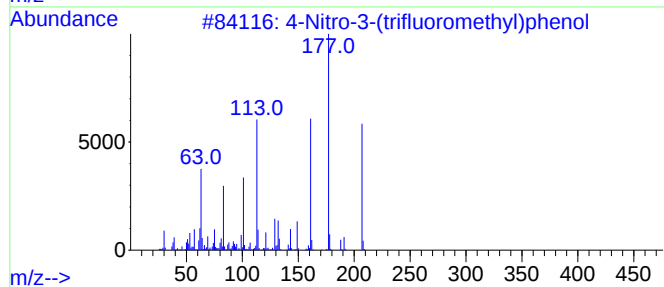
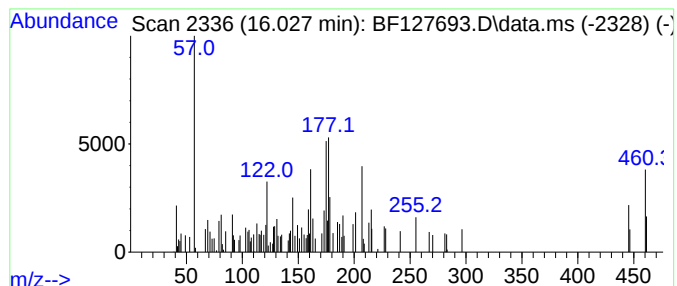
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.027 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	2.57 ng	106564	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Nitro-3-(trifluoromethyl)phenol	207	C7H4F3NO3	000088-30-2	38
2			3-Amino-2-carbomethoxybenzothiop...	207	C10H9NO2S	035212-85-2	18
3			2-Chloro-6-(trifluoromethyl)benz...	210	C8H6ClF3O	886500-21-6	18
4			5-Methylthiophene-2-sulfonamide	177	C5H7NO2S2	053595-69-0	18
5			Methyl cis-3-[p-anisido]acrylate	207	C11H13NO3	007542-88-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127693.D
Acq On : 07 Apr 2022 19:59
Operator : CG\JU
Sample : N2270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FARMINGDALE-CLAY-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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
Butane, 2-metho...	2.310	7.3	ng	260915	1	6.963	715837	20.0
Ethanol, 2-(2-b...	8.139	2.5	ng	114578	2	8.245	928497	20.0
unknown10.892	10.892	15.7	ng	920747	4	11.498	1173430	20.0
1-Heneicosanol	13.986	10.2	ng	476074	5	14.145	934446	20.0
Benzenepropanoi...	14.569	106.0	ng	4954340	5	14.145	934446	20.0
Tetracosane	14.857	3.4	ng	160065	5	14.145	934446	20.0
unknown16.027	16.027	2.6	ng	106564	6	15.674	827814	20.0