

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
 Data File : BF137739.D
 Acq On : 26 Apr 2024 17:21
 Operator : CG\JU
 Sample : P2271-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-3860

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-BF042324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137739.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	18	23	31	rVB2	61054	122399	1.51%	0.205%
2	2.446	55	61	70	rVB	499402	656318	8.08%	1.100%
3	3.728	272	279	294	rBV	307934	558708	6.88%	0.936%
4	5.687	607	612	615	rBV	6009021	5715448	70.39%	9.578%
5	6.669	773	779	782	rBV	5400286	5845535	71.99%	9.796%
6	6.869	810	813	819	rBV	126151	113867	1.40%	0.191%
7	7.057	842	845	849	rVB	1815515	1531102	18.86%	2.566%
8	7.622	935	941	944	rBV	3977991	3744935	46.12%	6.276%
9	7.857	978	981	984	rBV	163468	118295	1.46%	0.198%
10	8.345	1059	1064	1067	rBV	2380870	2054255	25.30%	3.443%
11	8.645	1111	1115	1123	rBV	211406	213621	2.63%	0.358%
12	9.416	1241	1246	1249	rBV	7470320	7046856	86.79%	11.809%
13	10.104	1359	1363	1366	rBV	2998805	2332427	28.73%	3.909%
14	10.198	1371	1379	1382	rBV	5749647	8119826	100.00%	13.608%
15	10.898	1493	1498	1501	rBV	4571406	4372478	53.85%	7.328%
16	11.598	1613	1617	1620	rBV	2789216	2432154	29.95%	4.076%
17	11.622	1620	1621	1625	rVV	666921	398209	4.90%	0.667%
18	11.675	1625	1630	1632	rVB	96867	101129	1.25%	0.169%
19	12.104	1699	1703	1706	rBV2	720453	696699	8.58%	1.168%
20	12.128	1706	1707	1712	rVB2	157384	110973	1.37%	0.186%
21	12.216	1718	1722	1724	rBV2	154711	153624	1.89%	0.257%
22	12.816	1820	1824	1828	rBV	1192661	963757	11.87%	1.615%
23	12.892	1833	1837	1842	rVV3	156387	154686	1.91%	0.259%
24	13.045	1857	1863	1869	rBV2	690826	771929	9.51%	1.294%
25	13.186	1883	1887	1890	rBV	7188979	6454938	79.50%	10.817%
26	14.010	2020	2027	2028	rBV4	61722	109905	1.35%	0.184%
27	14.074	2035	2038	2050	rVB2	295533	435144	5.36%	0.729%
28	14.210	2058	2061	2063	rBV	243409	199925	2.46%	0.335%
29	14.245	2063	2067	2070	rVV	1580689	1571190	19.35%	2.633%
30	14.274	2070	2072	2077	rVB	198273	182533	2.25%	0.306%
31	14.880	2171	2175	2181	rBV2	65891	109831	1.35%	0.184%
32	15.033	2197	2201	2207	rVB3	72840	139952	1.72%	0.235%
33	15.127	2213	2217	2223	rVB2	114940	141779	1.75%	0.238%
34	15.345	2249	2254	2257	rBV	132434	206019	2.54%	0.345%
35	15.680	2307	2311	2318	rVB	76763	100626	1.24%	0.169%
36	15.751	2318	2323	2329	rVV	77336	110637	1.36%	0.185%

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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_F\Methods\8270-BF042324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.821	2329	2335	2348	rVB	1117946	1495136	18.41%	2.506%
38	17.445	2606	2611	2620	rBV3	36714	84836	1.04%	0.142%

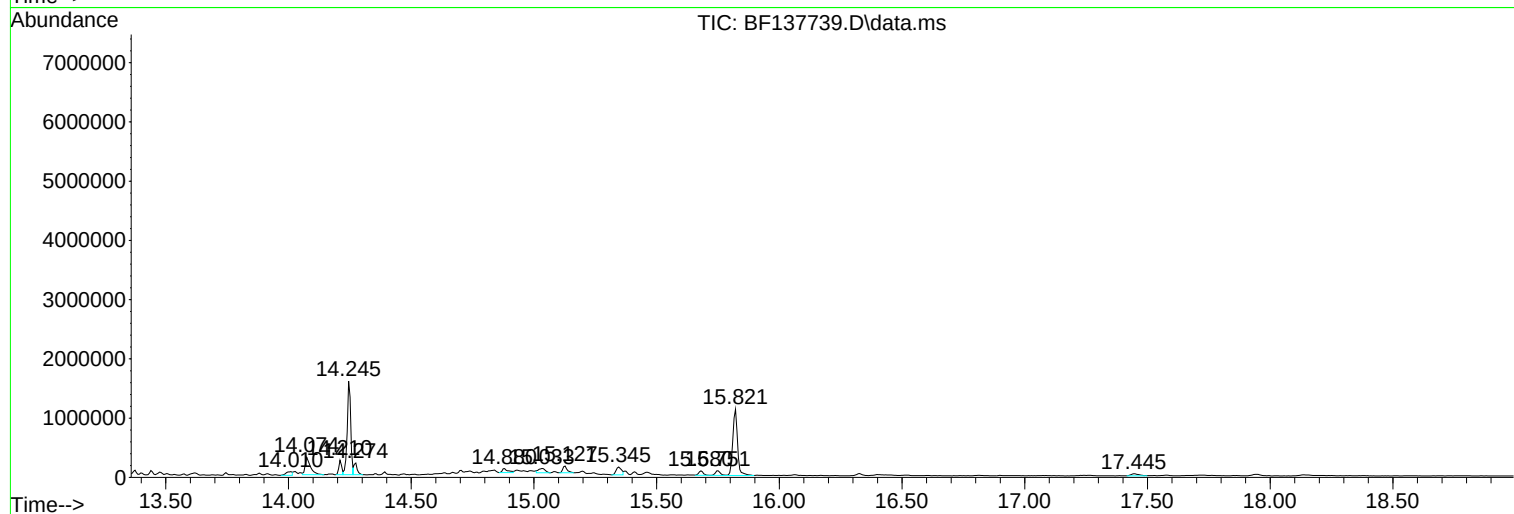
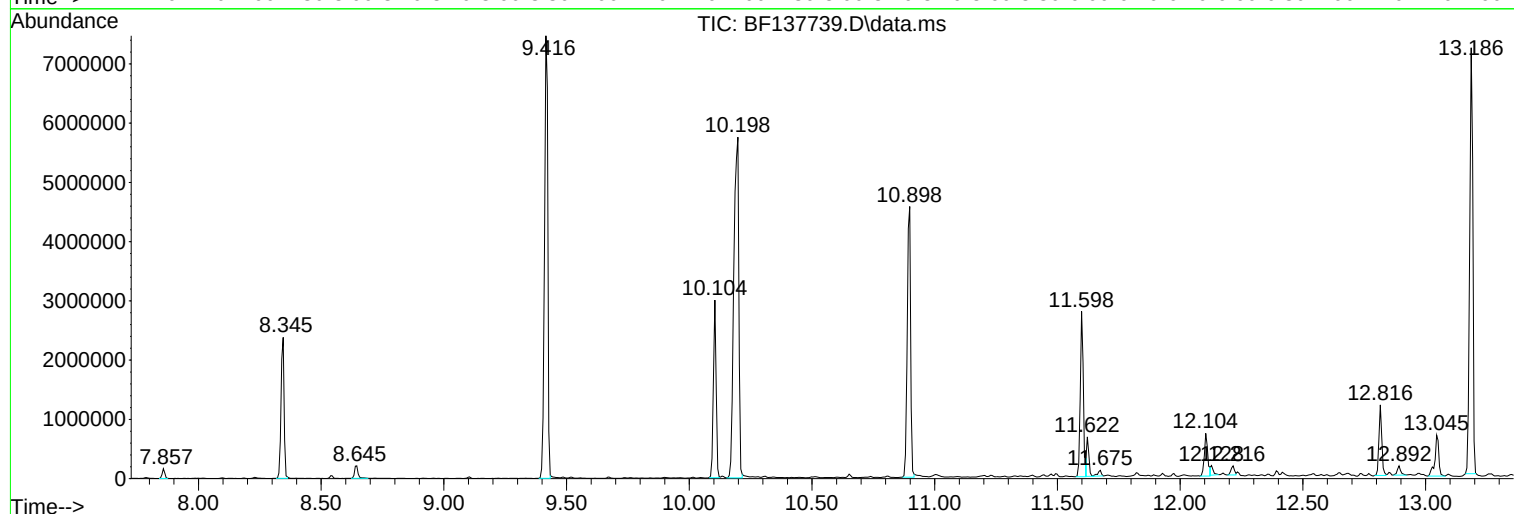
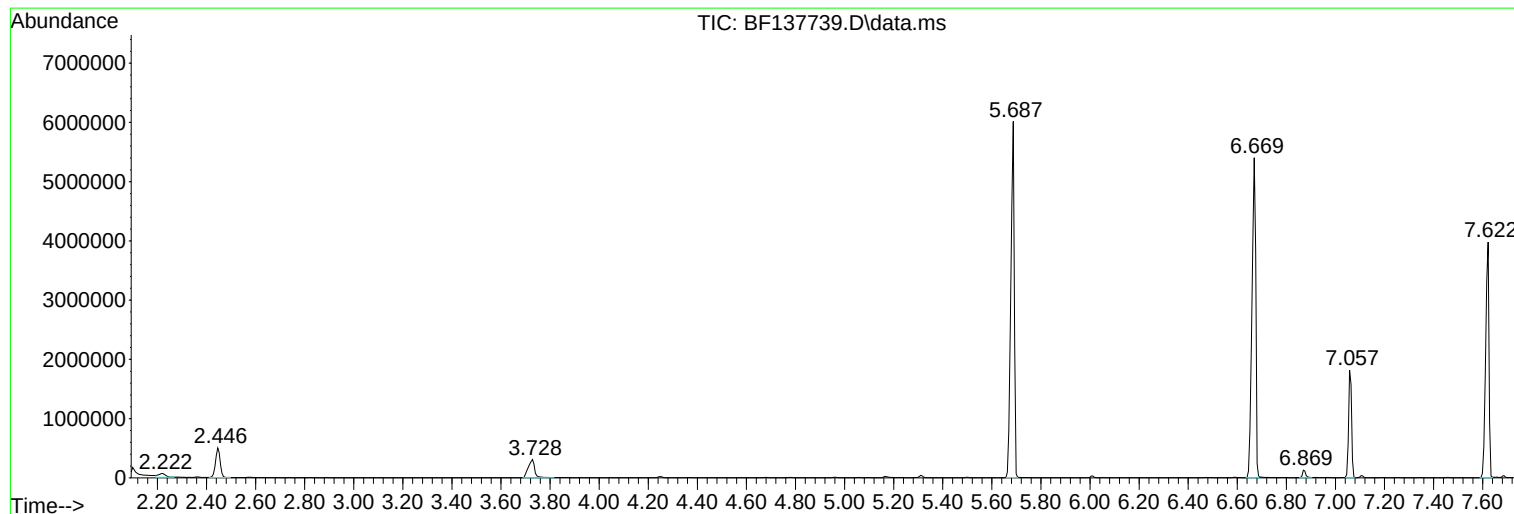
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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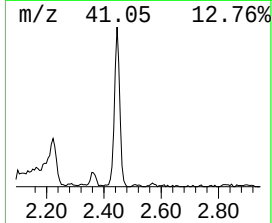
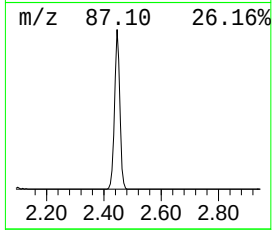
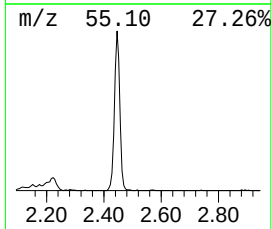
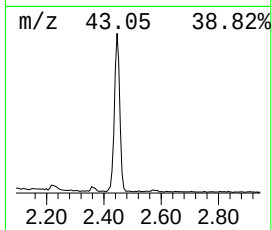
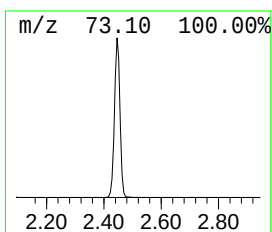
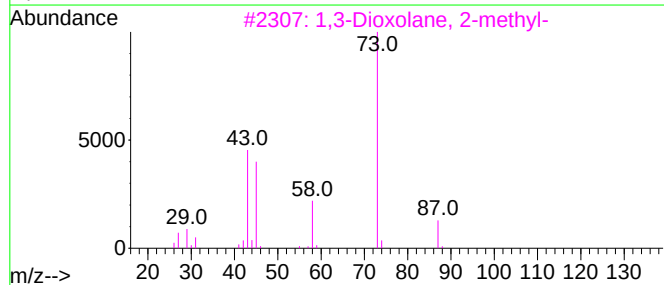
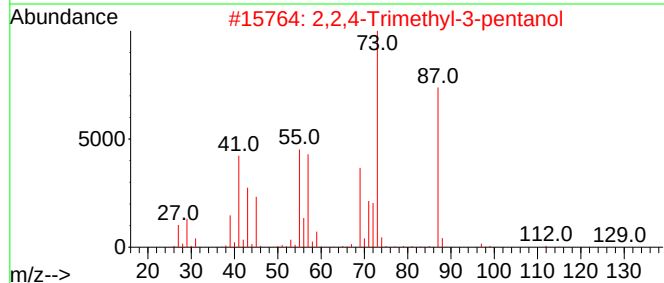
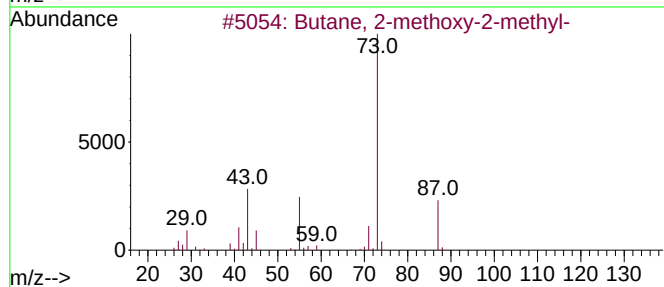
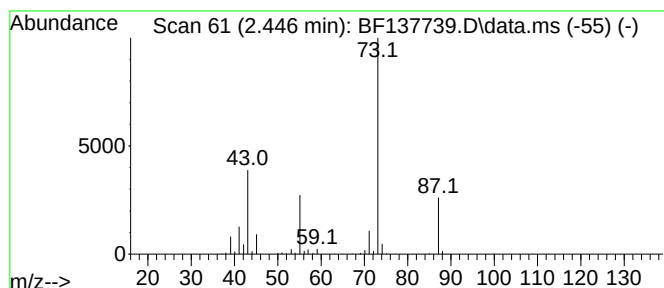
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.446	8.57 ng	656318	1,4-Dichlorobenzene-d4	7.057

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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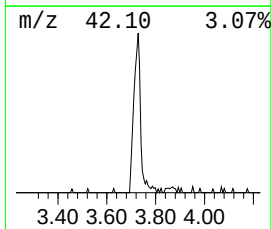
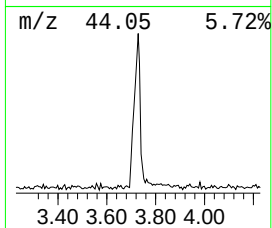
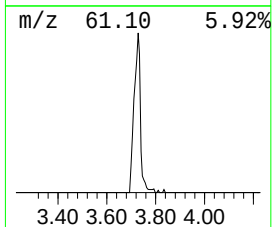
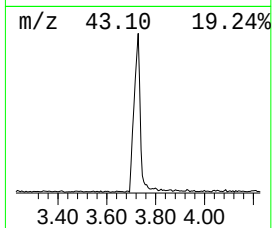
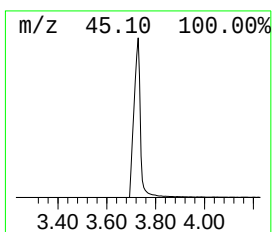
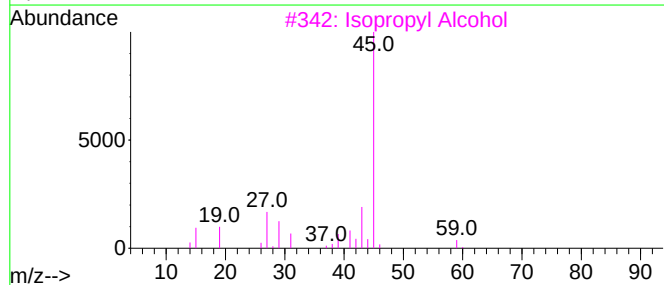
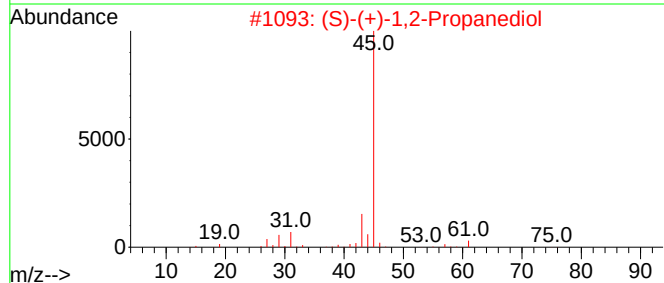
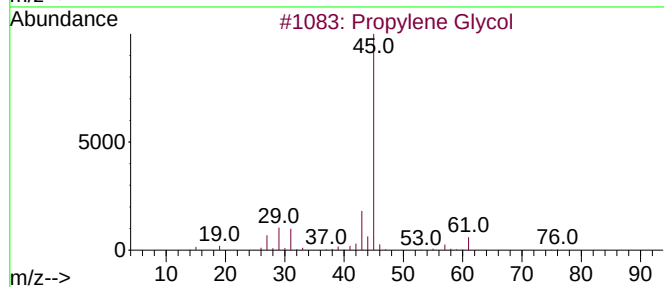
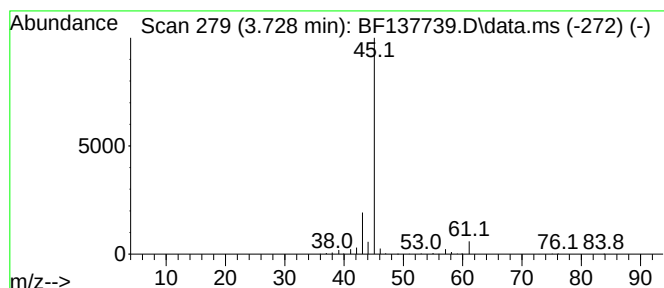
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.728	7.30 ng	558708	1,4-Dichlorobenzene-d4	7.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propylene Glycol	76	C3H8O2	000057-55-6	86
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40



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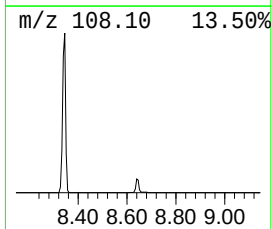
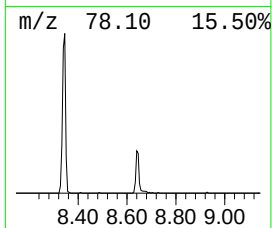
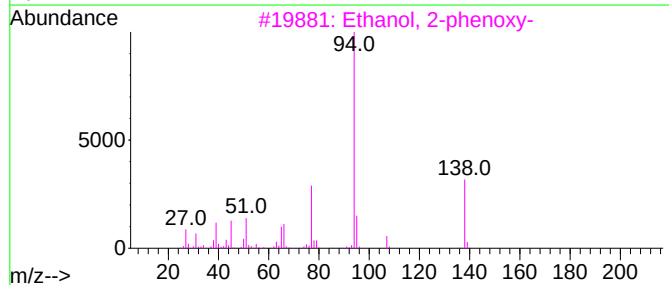
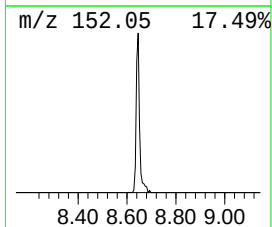
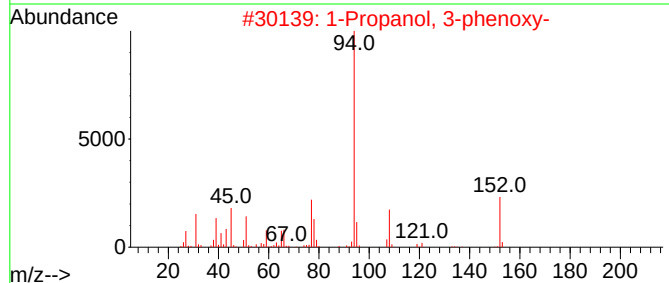
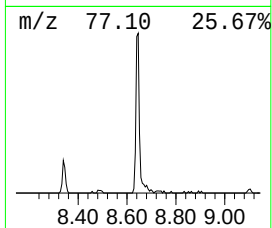
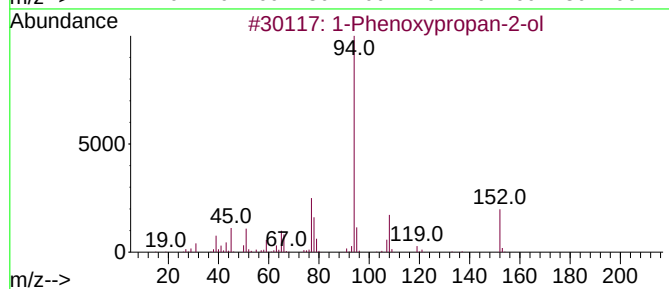
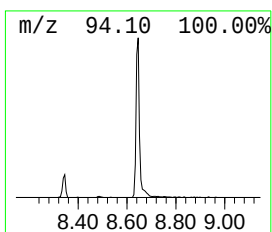
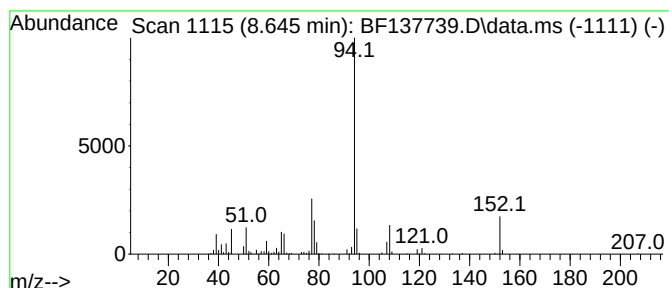
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.645	2.08 ng	213621	Naphthalene-d8	8.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			Pentanenitrile, 5-phenoxy-	175	C11H13NO	016728-56-6	53



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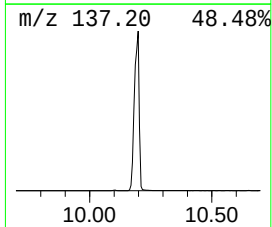
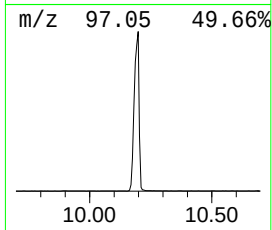
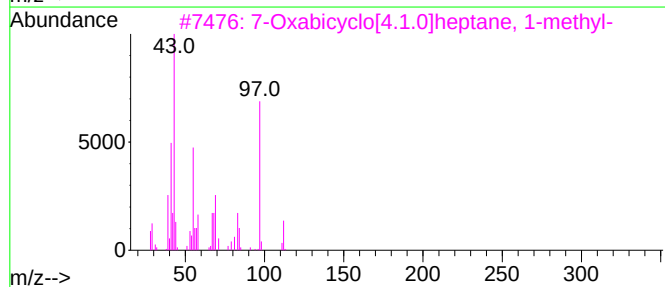
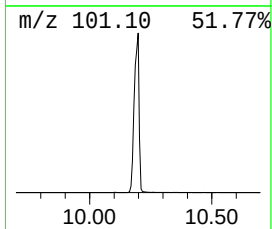
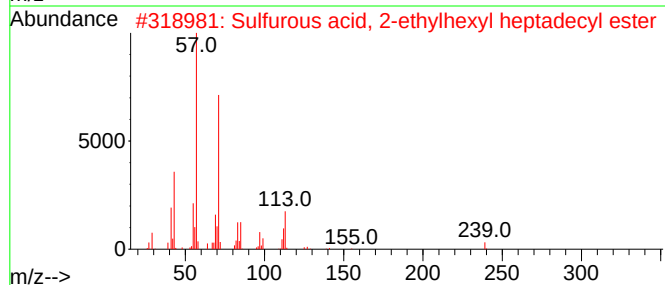
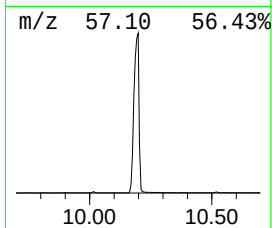
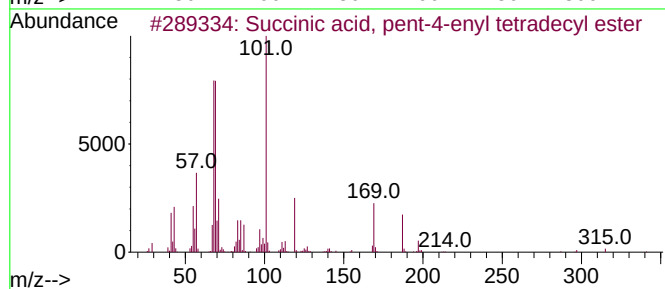
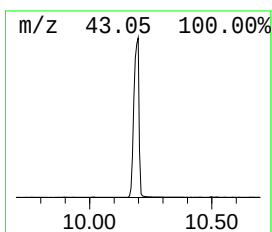
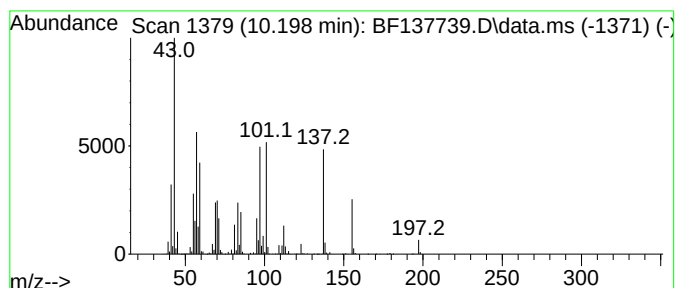
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown10.198 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.198	69.63 ng	8119830	Acenaphthene-d10	10.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, pent-4-enyl tetra...	382	C23H42O4	1000353-38-0	10
2			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	10
3			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	10
4			Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10
5			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10



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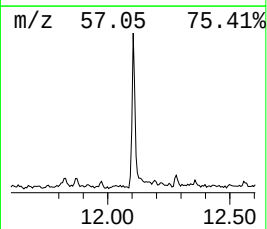
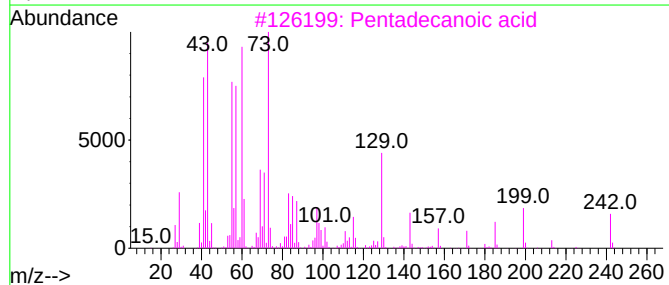
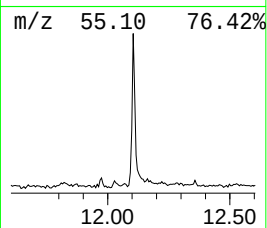
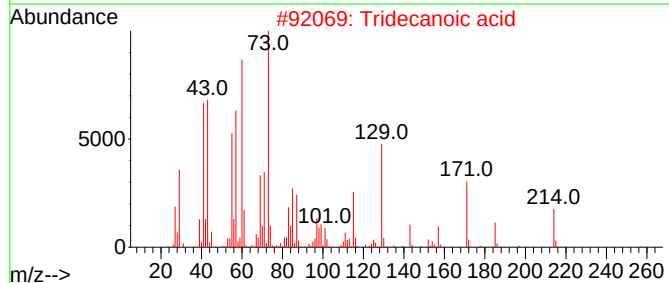
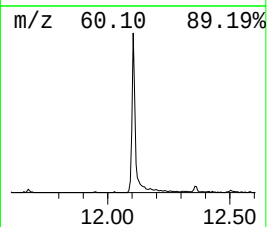
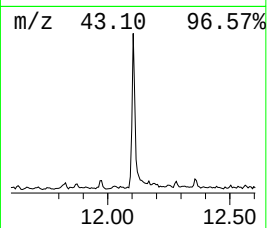
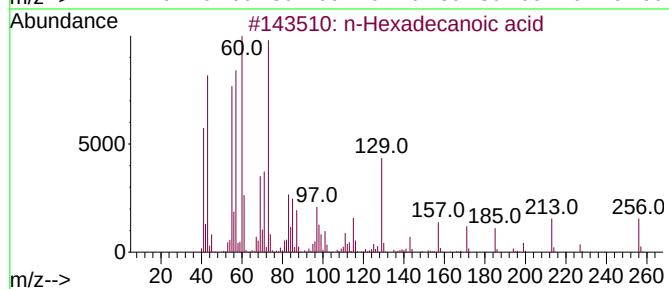
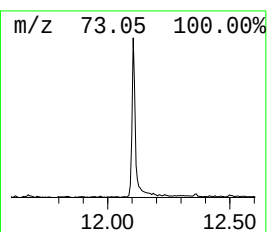
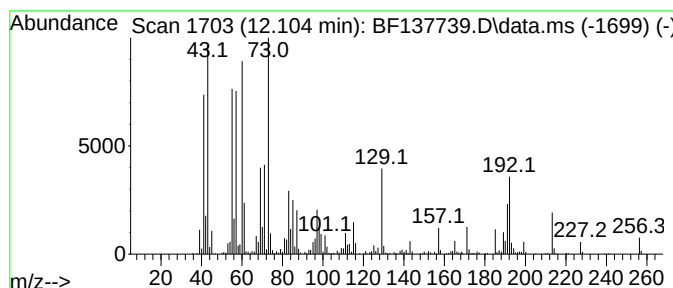
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	5.73 ng	696699	Phenanthrene-d10	11.598

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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Acq On : 26 Apr 2024 17:21
Operator : CG\JU
Sample : P2271-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3860

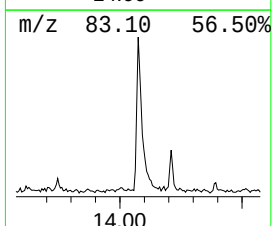
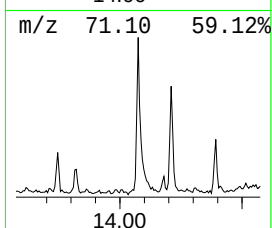
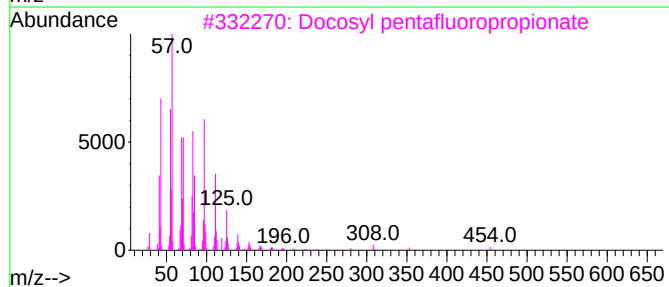
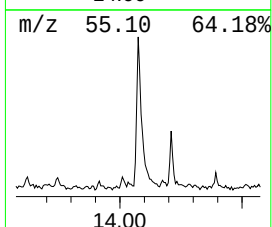
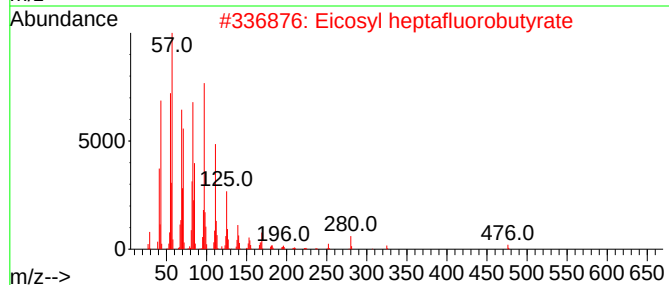
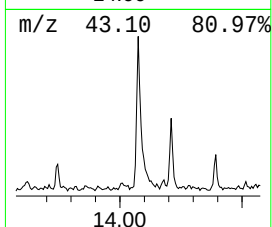
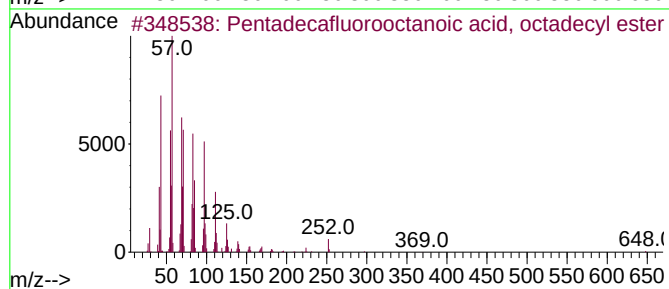
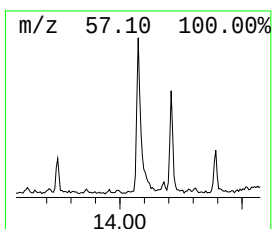
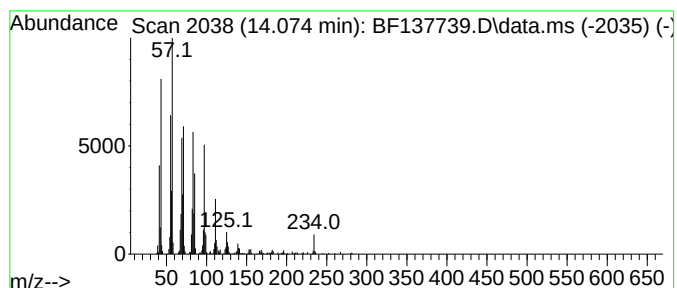
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	5.54 ng	435144	Chrysene-d12	14.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2		Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
4		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
5		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137739.D
Acq On : 26 Apr 2024 17:21
Operator : CG\JU
Sample : P2271-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3860

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.446	8.6	ng	656318	1	7.057	1531100	20.0
Propylene Glycol	3.728	7.3	ng	558708	1	7.057	1531100	20.0
1-Phenoxypropan...	8.645	2.1	ng	213621	2	8.345	2054260	20.0
unknown10.198	10.198	69.6	ng	8119830	3	10.104	2332430	20.0
n-Hexadecanoic ...	12.104	5.7	ng	696699	4	11.598	2432150	20.0
Pentadecafluoro...	14.074	5.5	ng	435144	5	14.245	1571190	20.0