

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031324\
 Data File : BF137580.D
 Acq On : 13 Mar 2024 16:54
 Operator : CG\JU
 Sample : P1733-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	29	39	56	rVB	1151506	1635229	30.33%	4.015%
2	5.604	593	598	601	rBV	4781725	4630899	85.89%	11.371%
3	6.569	757	762	765	rBV	4423709	4875302	90.42%	11.972%
4	6.922	819	822	832	rBV	1438244	1272069	23.59%	3.124%
5	7.481	912	917	920	rBV	3269636	3087927	57.27%	7.583%
6	8.192	1034	1038	1055	rBV	1814171	1756378	32.57%	4.313%
7	9.269	1216	1221	1224	rBV	5879528	5391899	100.00%	13.240%
8	9.386	1237	1241	1245	rBV	887236	843401	15.64%	2.071%
9	9.945	1332	1336	1340	rBV	2229743	1993487	36.97%	4.895%
10	10.051	1350	1354	1360	rVB	59576	79947	1.48%	0.196%
11	10.745	1467	1472	1490	rBV	3196271	3324057	61.65%	8.162%
12	11.445	1587	1591	1594	rBV	1946109	1831215	33.96%	4.497%
13	11.992	1679	1684	1694	rBV3	230772	347641	6.45%	0.854%
14	12.563	1775	1781	1784	rBV3	87482	83768	1.55%	0.206%
15	12.663	1793	1798	1804	rBV	136799	155136	2.88%	0.381%
16	12.892	1832	1837	1841	rBV	123160	151593	2.81%	0.372%
17	13.051	1859	1864	1867	rBV	5015776	4906985	91.01%	12.049%
18	13.286	1898	1904	1909	rBV2	58232	70846	1.31%	0.174%
19	13.539	1942	1947	1954	rBV	289480	330283	6.13%	0.811%
20	13.633	1959	1963	1966	rVV2	65090	64468	1.20%	0.158%
21	13.962	2015	2019	2029	rBV	307206	403200	7.48%	0.990%
22	14.104	2038	2043	2047	rBV2	1488427	1602170	29.71%	3.934%
23	14.286	2071	2074	2077	rBV	71042	60174	1.12%	0.148%
24	14.598	2124	2127	2131	rBV	64812	70152	1.30%	0.172%
25	15.015	2194	2198	2206	rVB	165610	194220	3.60%	0.477%
26	15.204	2226	2230	2240	rBV	53943	112938	2.09%	0.277%
27	15.315	2245	2249	2255	rBV2	49883	61548	1.14%	0.151%
28	15.604	2294	2298	2305	rBV	39389	59758	1.11%	0.147%
29	15.674	2305	2310	2319	rBV	917603	1327177	24.61%	3.259%

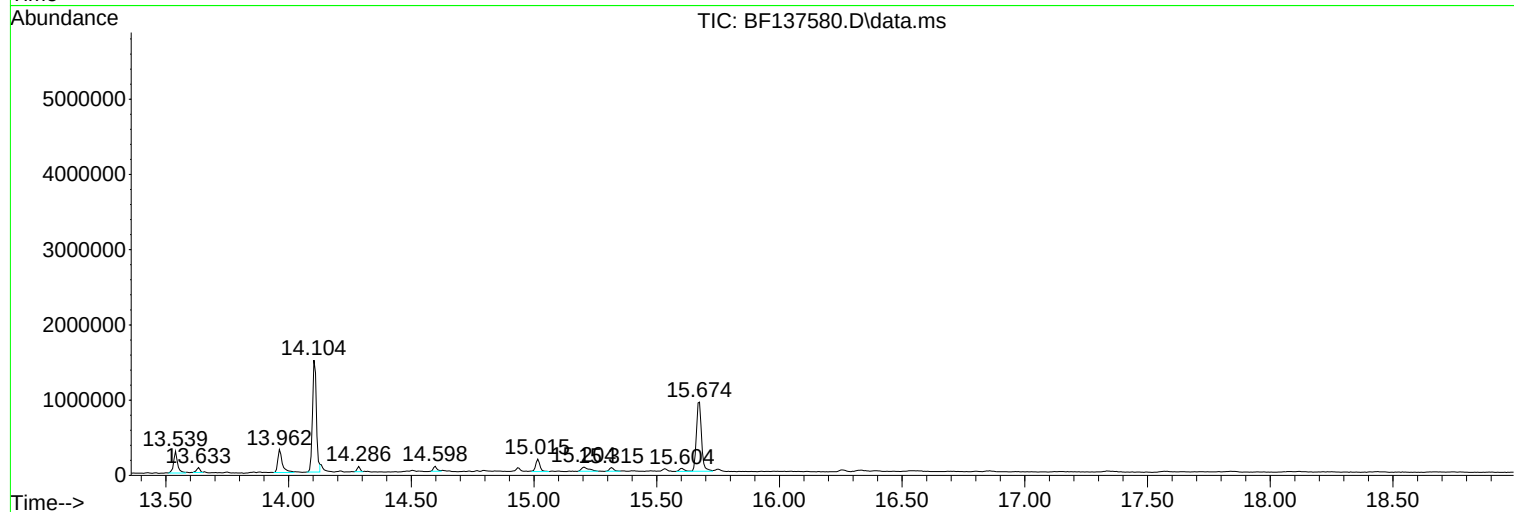
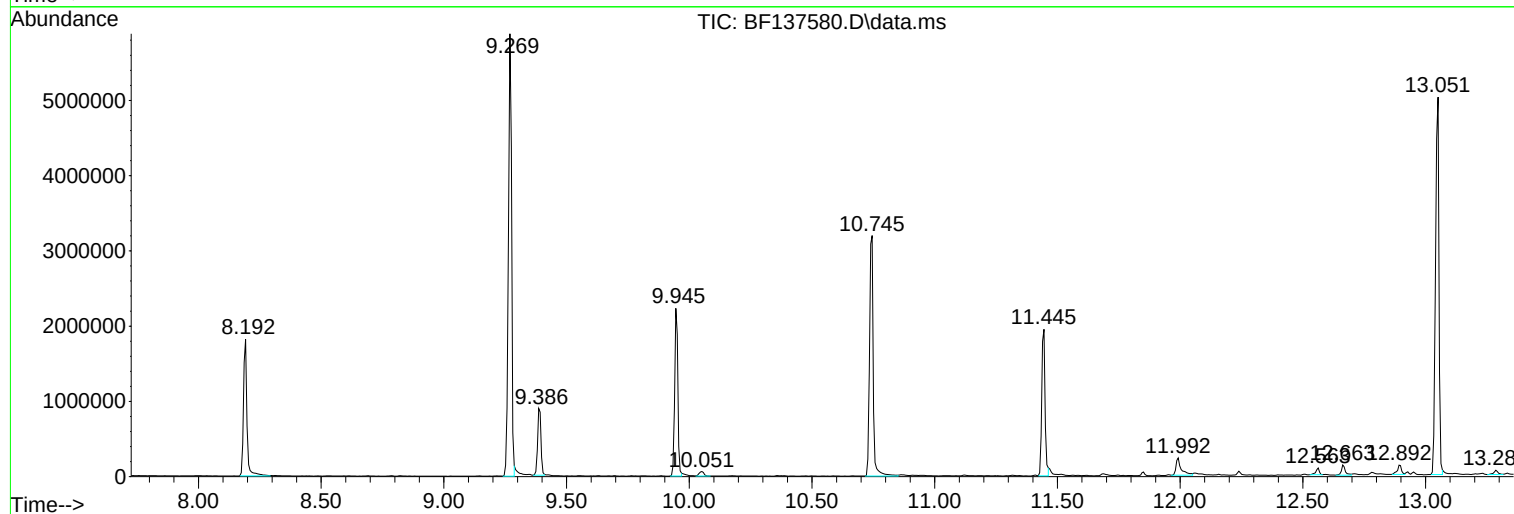
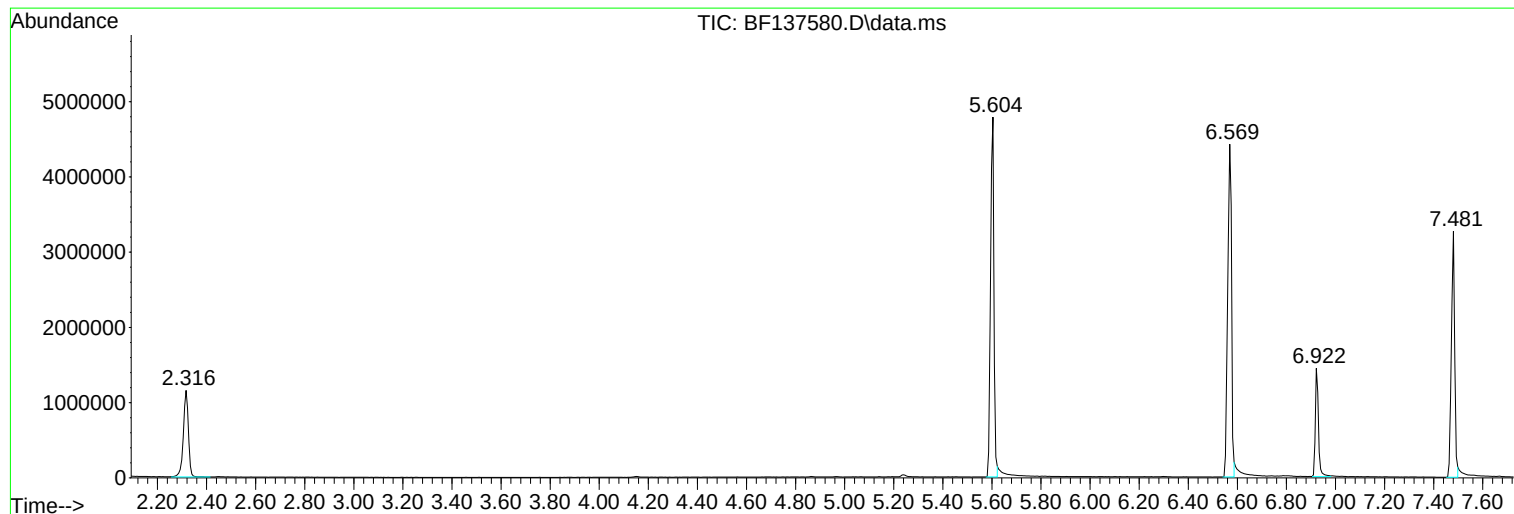
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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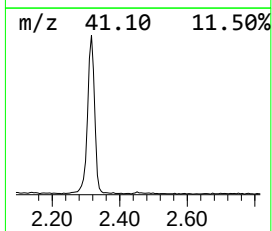
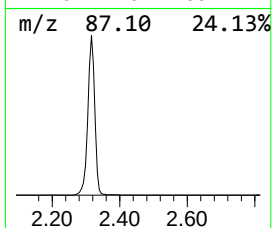
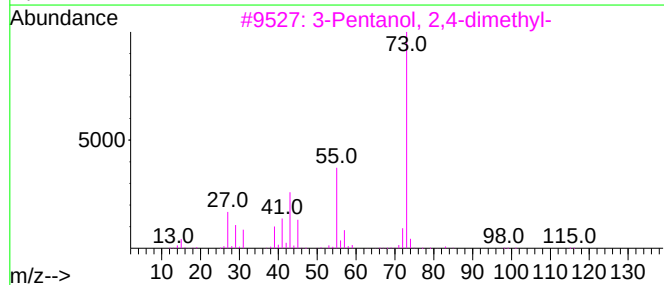
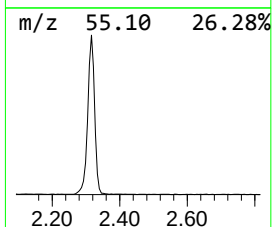
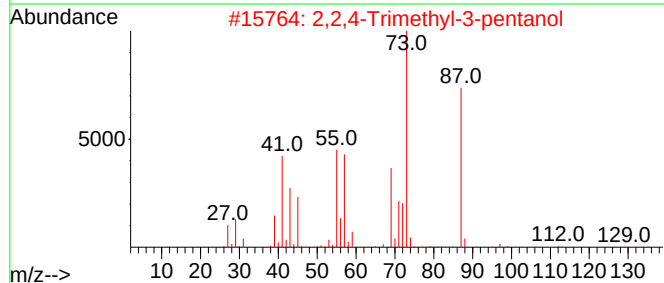
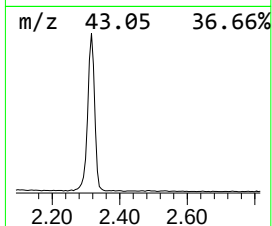
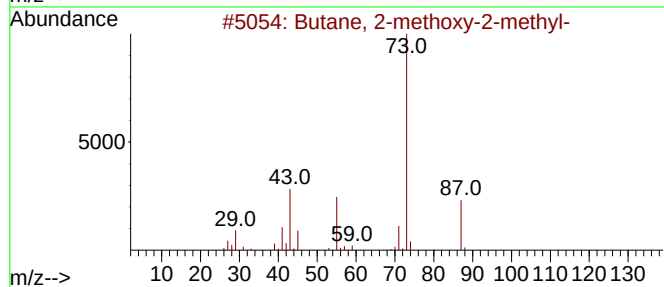
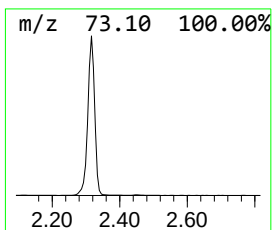
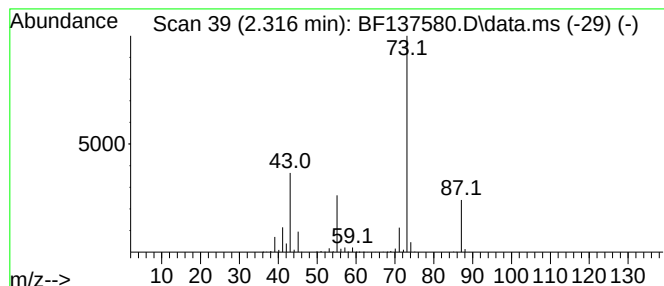
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.316	25.71 ng	1635230	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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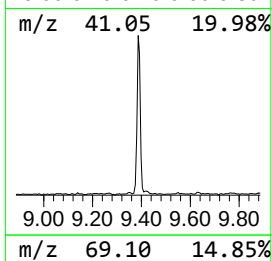
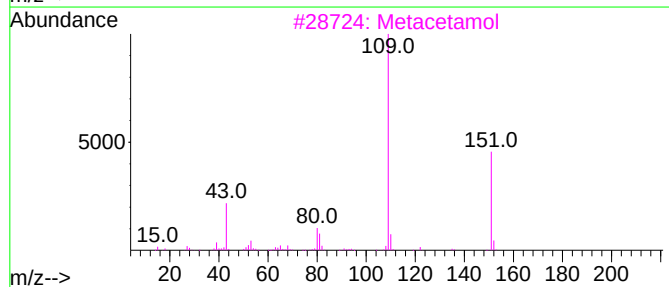
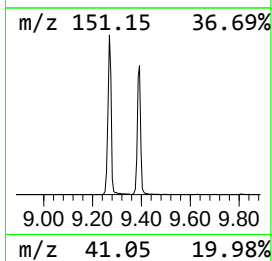
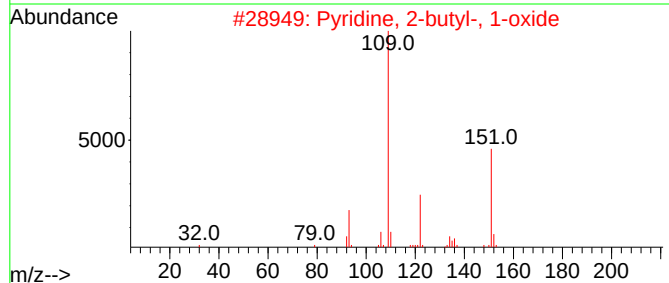
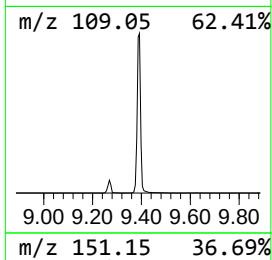
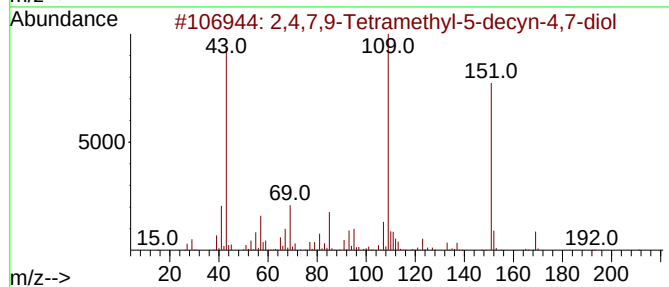
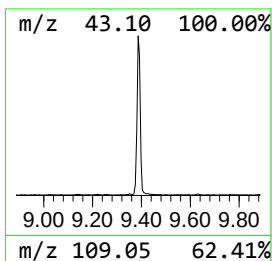
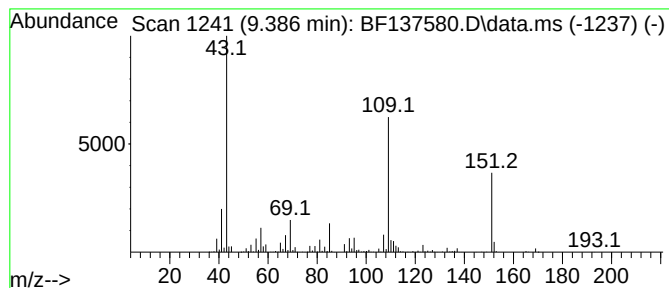
Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.386	8.46 ng	843401	Acenaphthene-d10		9.945	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	53
3	Metacetamol		151	C8H9NO2	000621-42-1	47
4	3-Pyridinol, 4-methyl-, acetate ...		151	C8H9NO2	001006-96-8	47
5	(-)-10-Camphorsulfonyl chloride		250	C10H15ClO3S	039262-22-1	45



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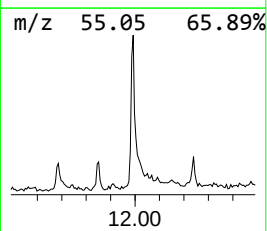
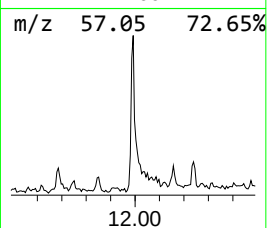
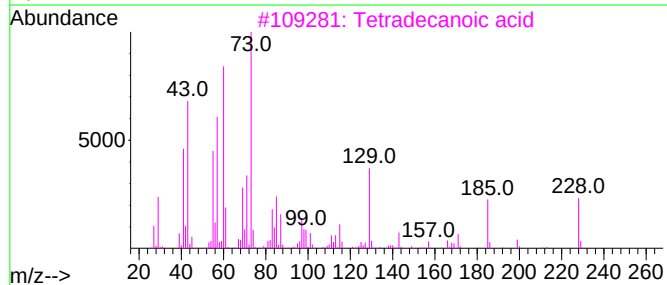
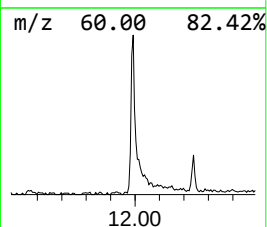
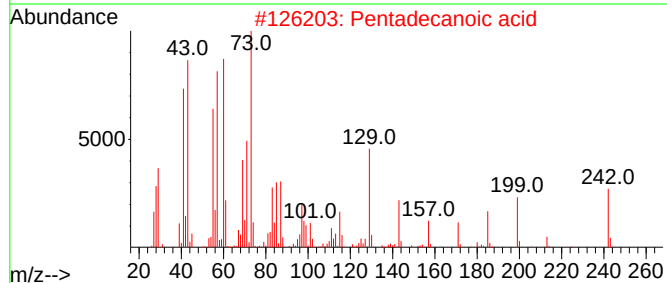
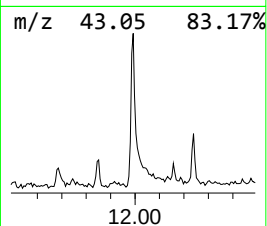
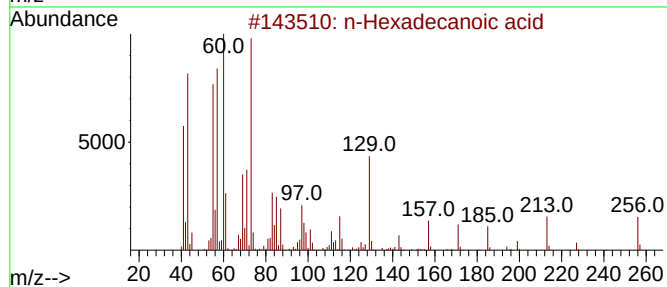
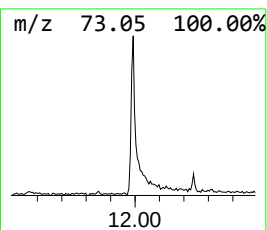
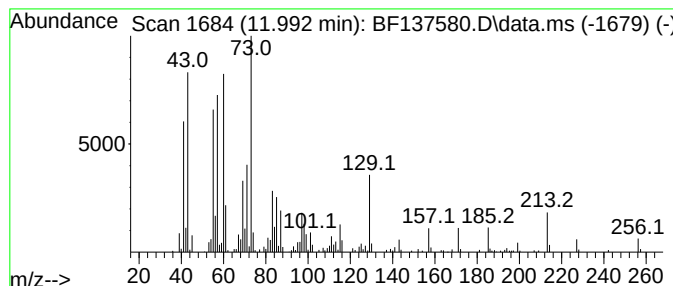
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.992	3.80 ng	347641	Phenanthrene-d10		11.445	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	94
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	94
4	Tridecanoic acid		214	C13H26O2	000638-53-9	81
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	60



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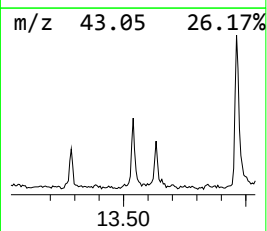
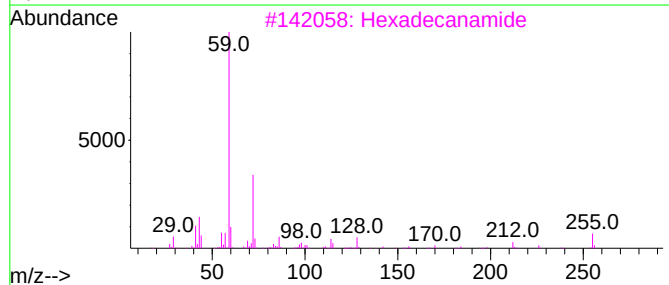
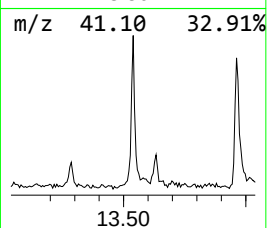
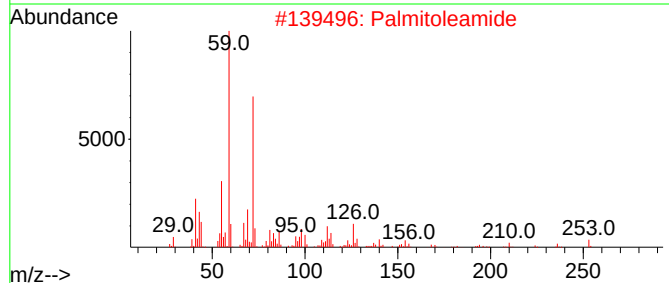
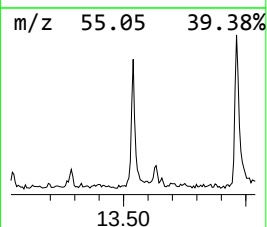
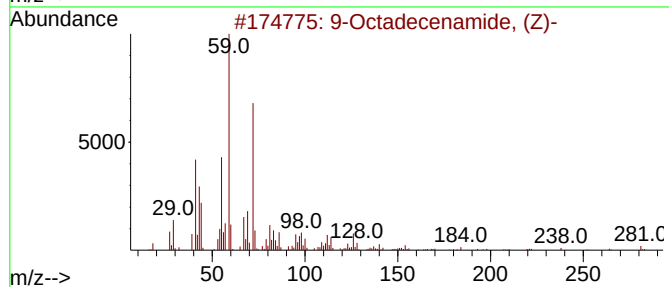
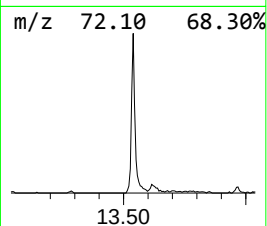
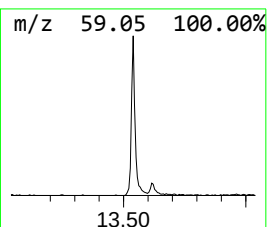
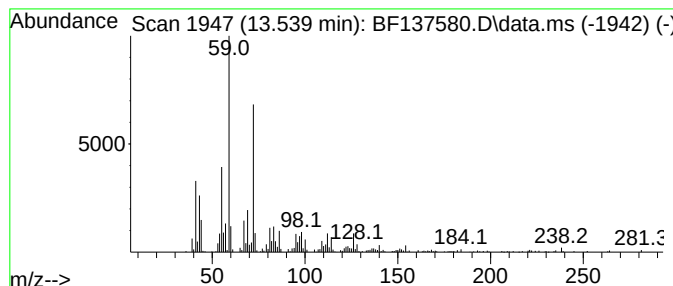
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.539	4.12 ng	330283	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2			Palmitoleamide	253	C16H31NO	106010-22-4	64
3			Hexadecanamide	255	C16H33NO	000629-54-9	56
4			Nonanamide	157	C9H19NO	001120-07-6	53
5			2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	43



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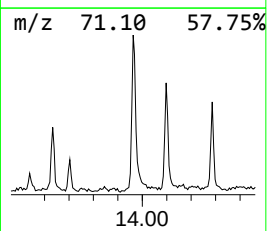
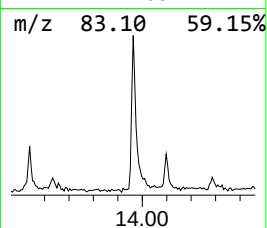
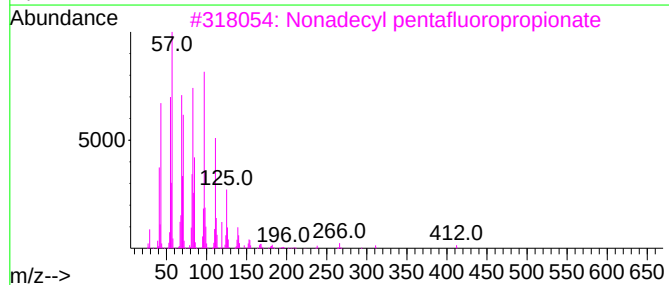
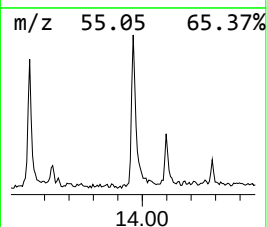
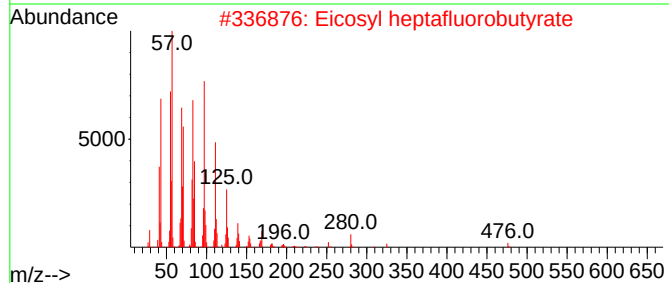
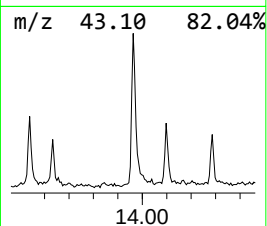
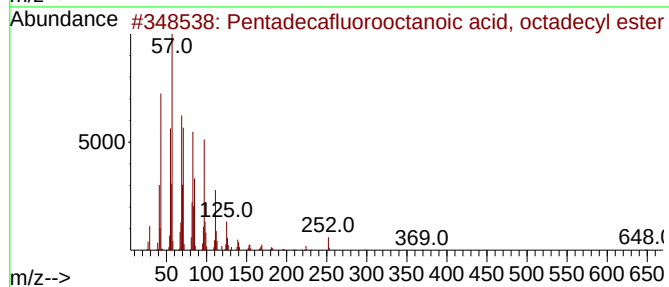
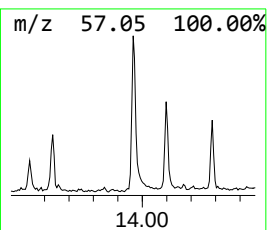
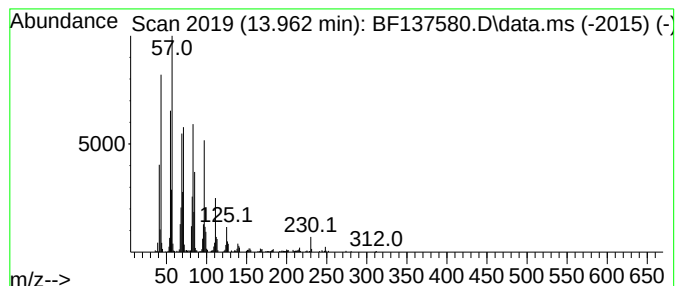
Instrument :
BNA_F
ClientSampleId :
WC-2

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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.963	5.03 ng	403200	Chrysene-d12	14.104	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90



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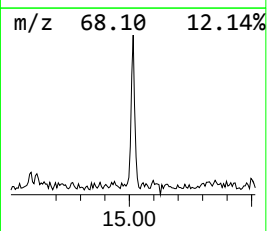
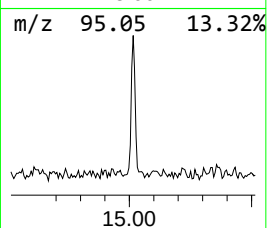
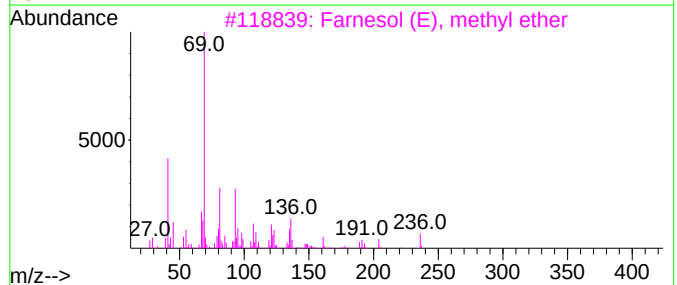
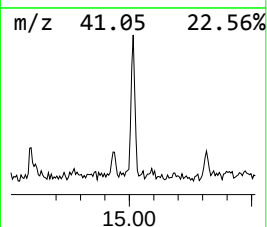
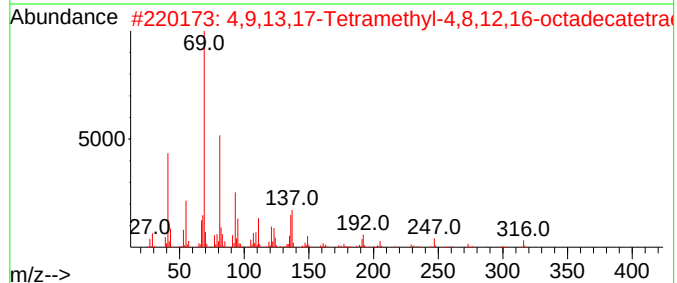
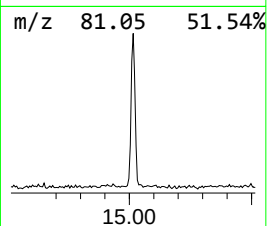
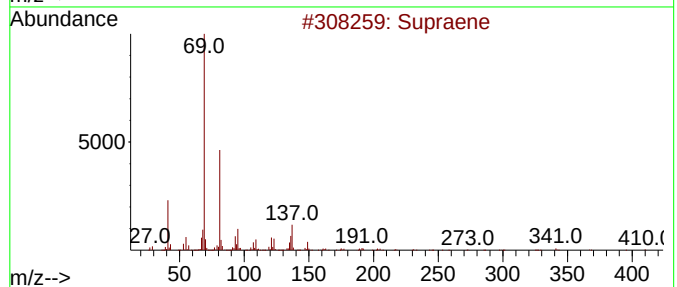
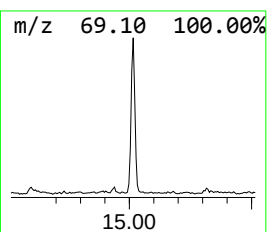
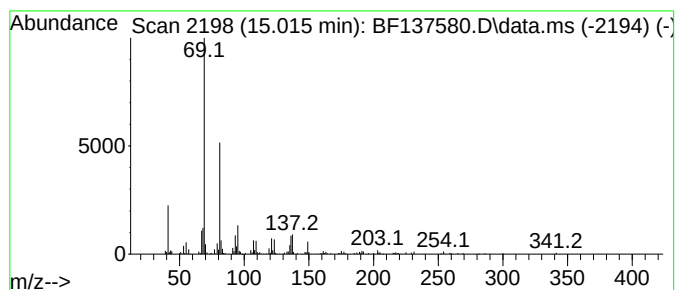
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.015	2.93 ng	194220	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3			Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031324\
Data File : BF137580.D
Acq On : 13 Mar 2024 16:54
Operator : CG\JU
Sample : P1733-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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...	2.316	25.7	ng	1635230	1	6.922	1272070	20.0
2,4,7,9-Tetrame...	9.386	8.5	ng	843401	3	9.945	1993490	20.0
n-Hexadecanoic ...	11.992	3.8	ng	347641	4	11.445	1831220	20.0
9-Octadecenamid...	13.539	4.1	ng	330283	5	14.104	1602170	20.0
Pentadecafluoro...	13.963	5.0	ng	403200	5	14.104	1602170	20.0
Supraene	15.015	2.9	ng	194220	6	15.674	1327180	20.0