LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111524\
Data File : BF140408.D
Acq On : 15 Nov 2024 17:13
Operator : RC/JU
Sample : P4807-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BF-F13

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-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140408.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	4	11	22	rVB	807115	1244317	47.80%	6.118%
2	5.093	500	510	523	rVB	38067	62134	2.39%	0.306%
3	5.504	575	580	601	rBV	1579138	2099310	80.65%	10.322%
4	6.510	745	751	769	rBV	1700553	2330170	89.52%	11.458%
5	6.875	807	813	818	rBV	614607	774909	29.77%	3.810%
6	7.434	902	908	916	rBV	1021309	1349405	51.84%	6.635%
7	7.510	916	921	935	rVB	53097	78003	3.00%	0.384%
8	7.681	946	950	963	rBV	40941	59805	2.30%	0.294%
9	8.151	1025	1030	1048	rVB	762831	998359	38.36%	4.909%
10	9.228	1207	1213	1235	rBV	1993356	2602916	100.00%	12.799%
11	9.910	1323	1329	1343	rVB	861343	1113374	42.77%	5.475%
12	10.622	1445	1450	1458	rBV	141110	174698	6.71%	0.859%
13	10.698	1458	1463	1479	rBV	1141374	1507382	57.91%	7.412%
14	11.398	1577	1582	1589	rBV	910126	1140277	43.81%	5.607%
15	11.922	1666	1671	1693	rBV2	119644	226396	8.70%	1.113%
16	12.498	1764	1769	1783	rVB	66325	98073	3.77%	0.482%
17	12.710	1800	1805	1812	rBV2	17899	35181	1.35%	0.173%
18	12.980	1846	1851	1857	rBV	1648969	2176077	83.60%	10.700%
19	13.910	2002	2009	2025	rBV6	25707	116853	4.49%	0.575%
20	14.051	2026	2033	2047	rVB	511559	733688	28.19%	3.608%
21	14.839	2162	2167	2175	rBV	431178	661126	25.40%	3.251%
22	15.568	2285	2291	2305	rBV	446070	754961	29.00%	3.712%

Sum of corrected areas: 20337414

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ClientSampleId :
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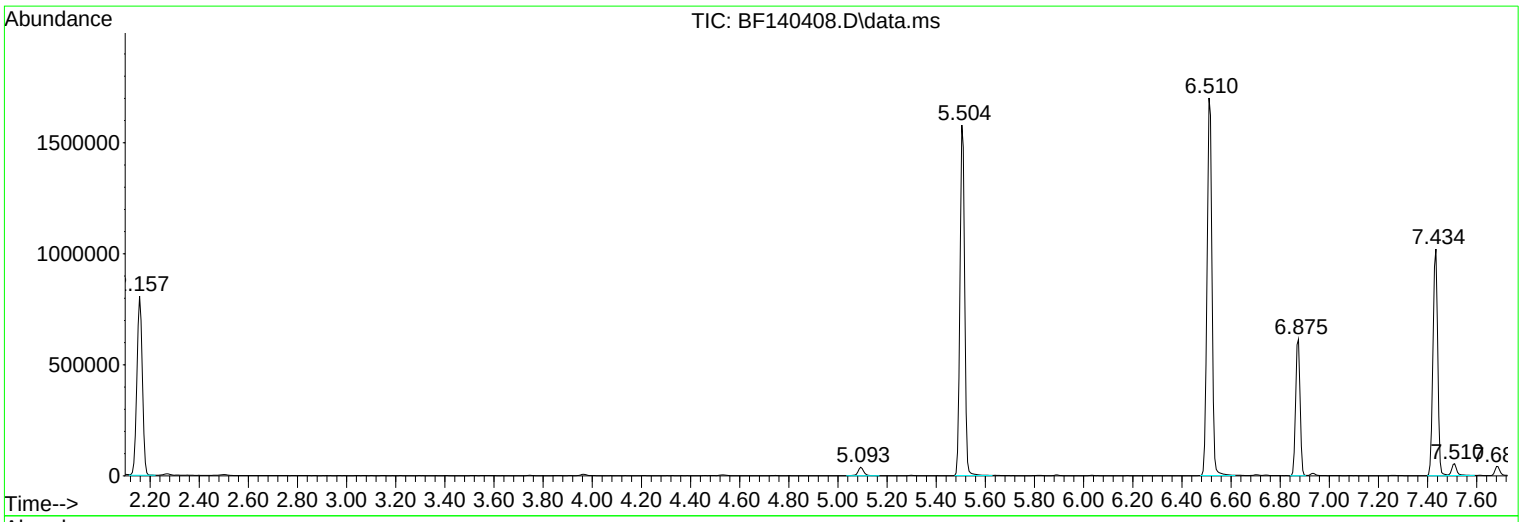
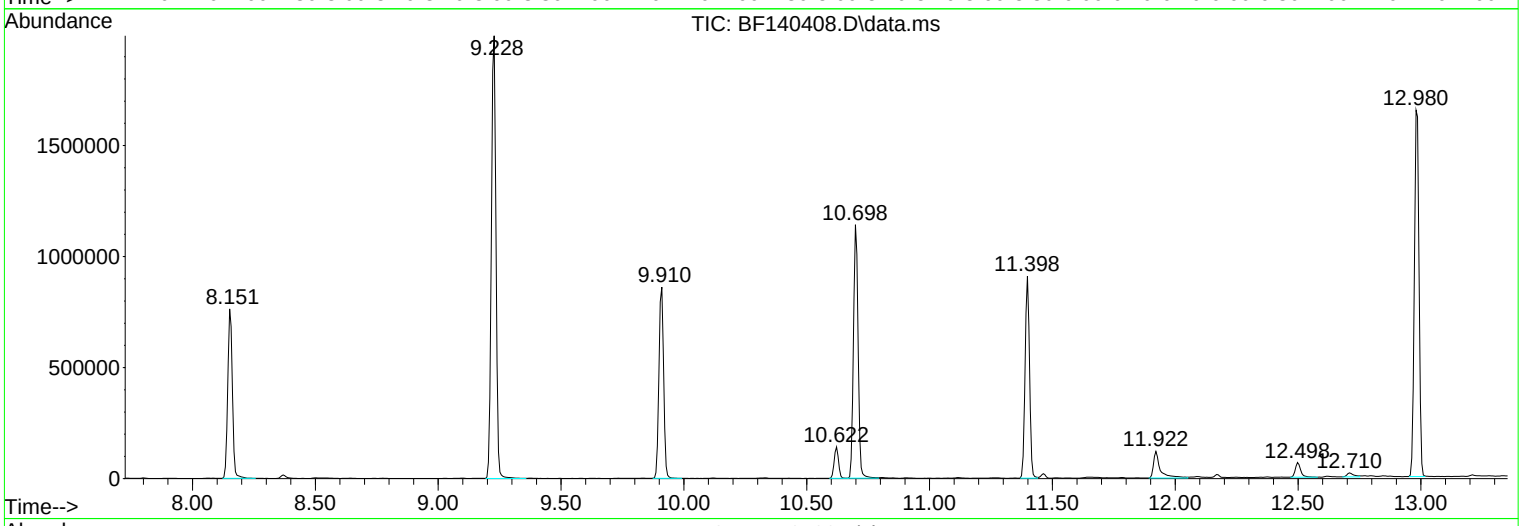
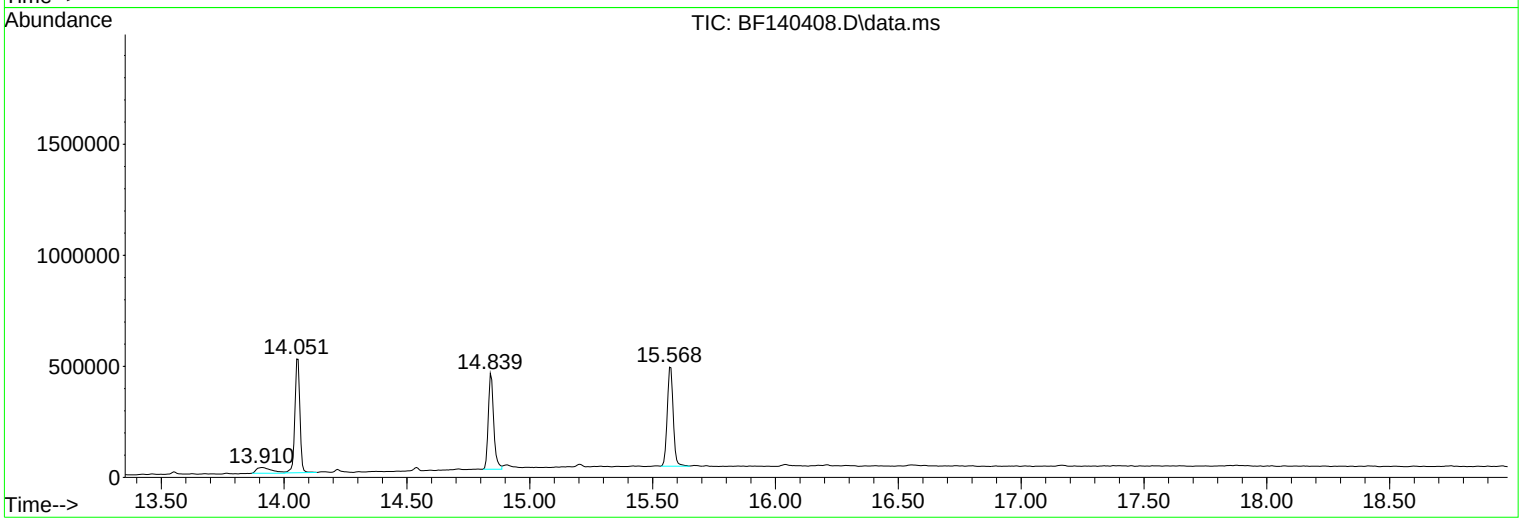
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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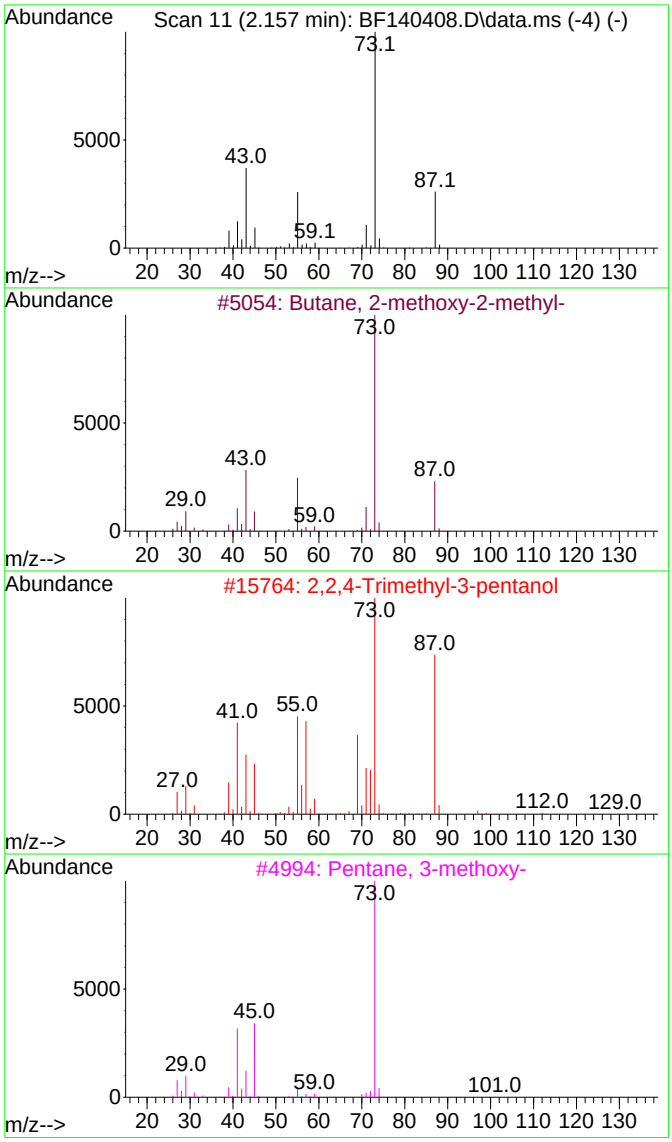
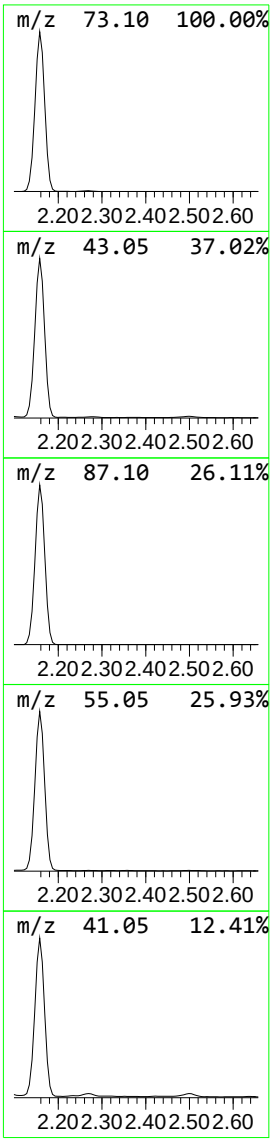
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	32.12 ng	1244320	1,4-Dichlorobenzene-d4	6.875

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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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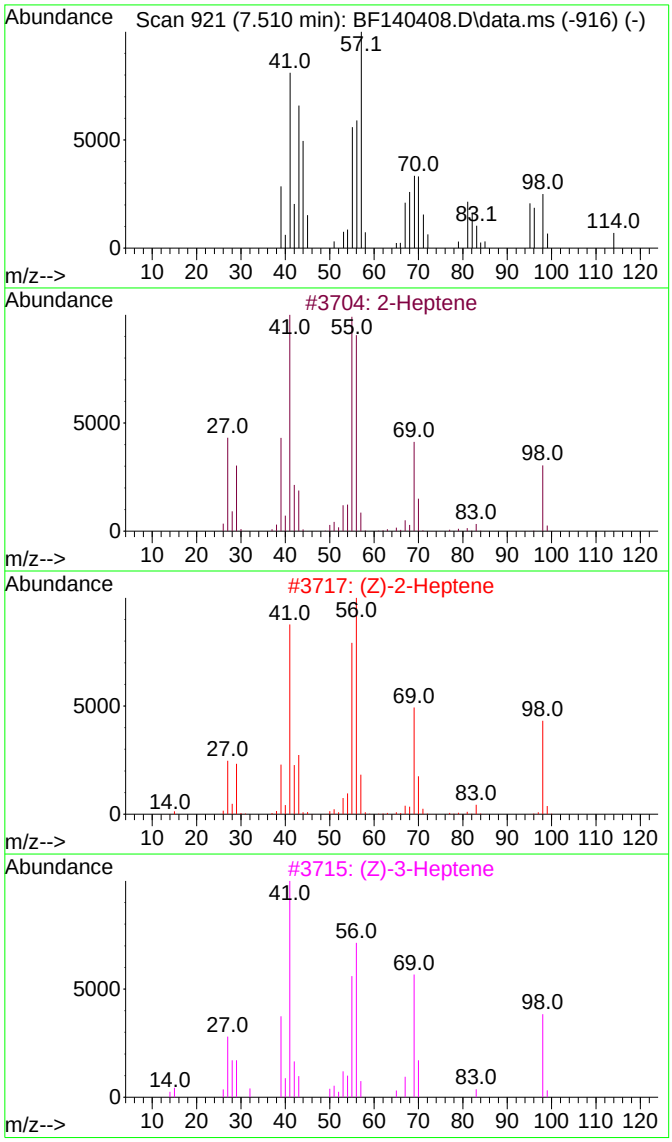
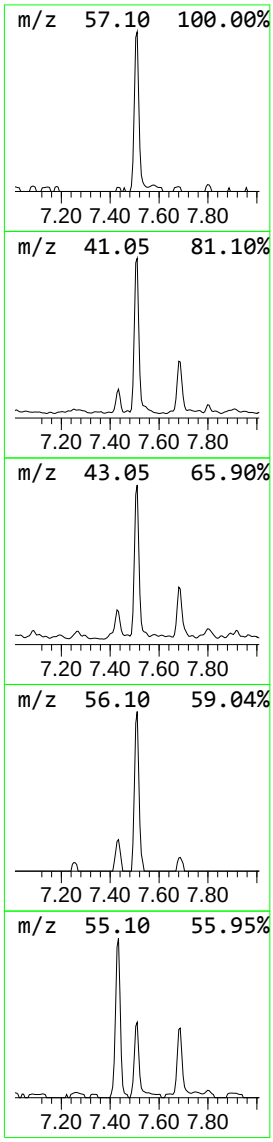
Peak Number 2 unknown7.510 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.510	2.01 ng	78003	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptene	98	C7H14	000592-77-8	35
2	(Z)-2-Heptene	98	C7H14	006443-92-1	30
3	(Z)-3-Heptene	98	C7H14	007642-10-6	25
4	2-Heptene, (E)-	98	C7H14	014686-13-6	25
5	3-Heptene	98	C7H14	000592-78-9	25





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ClientSampleId :
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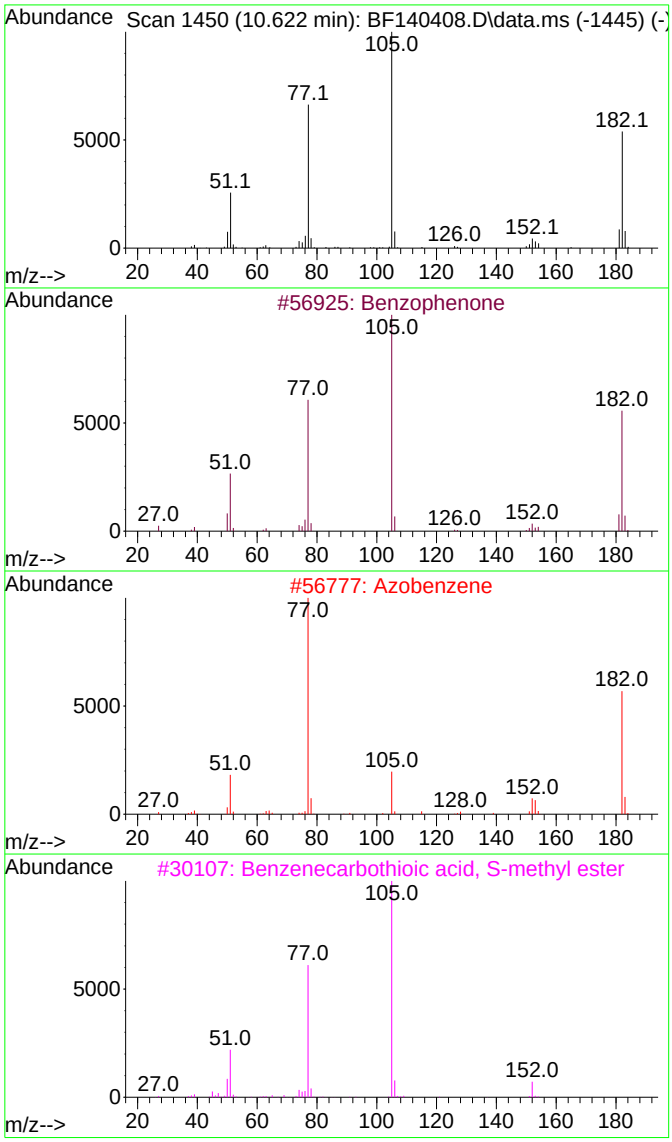
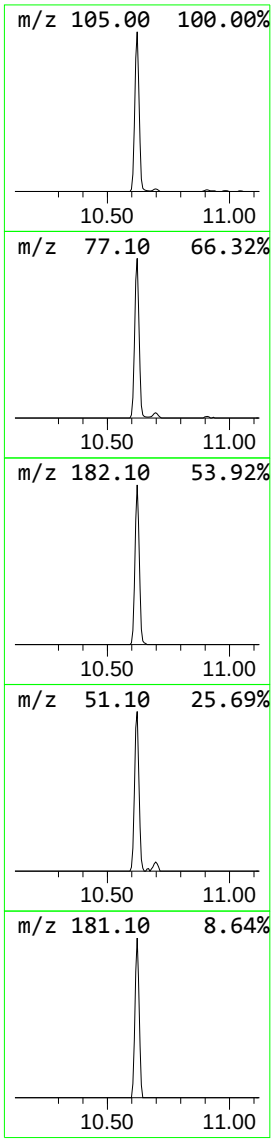
Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	3.14 ng	174698	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47





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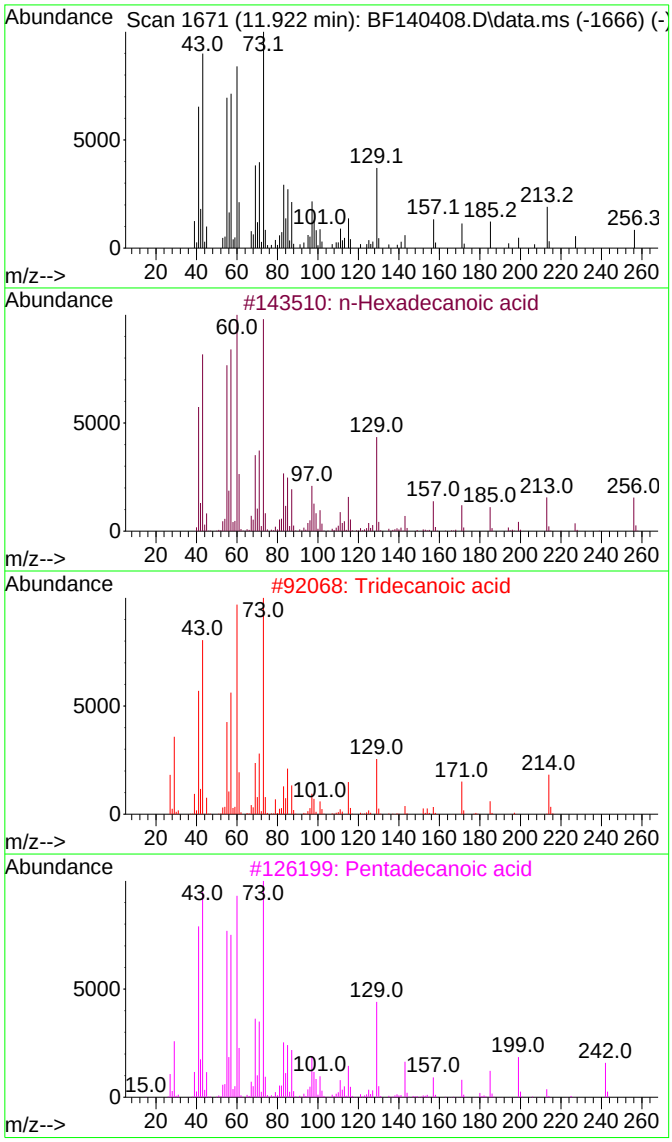
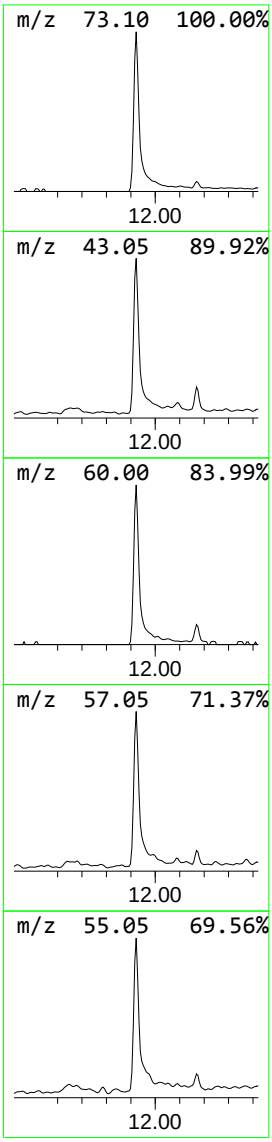
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.97 ng	226396	Phenanthrene-d10	11.398

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	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Nonanoic acid	158	C9H18O2	000112-05-0	45





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Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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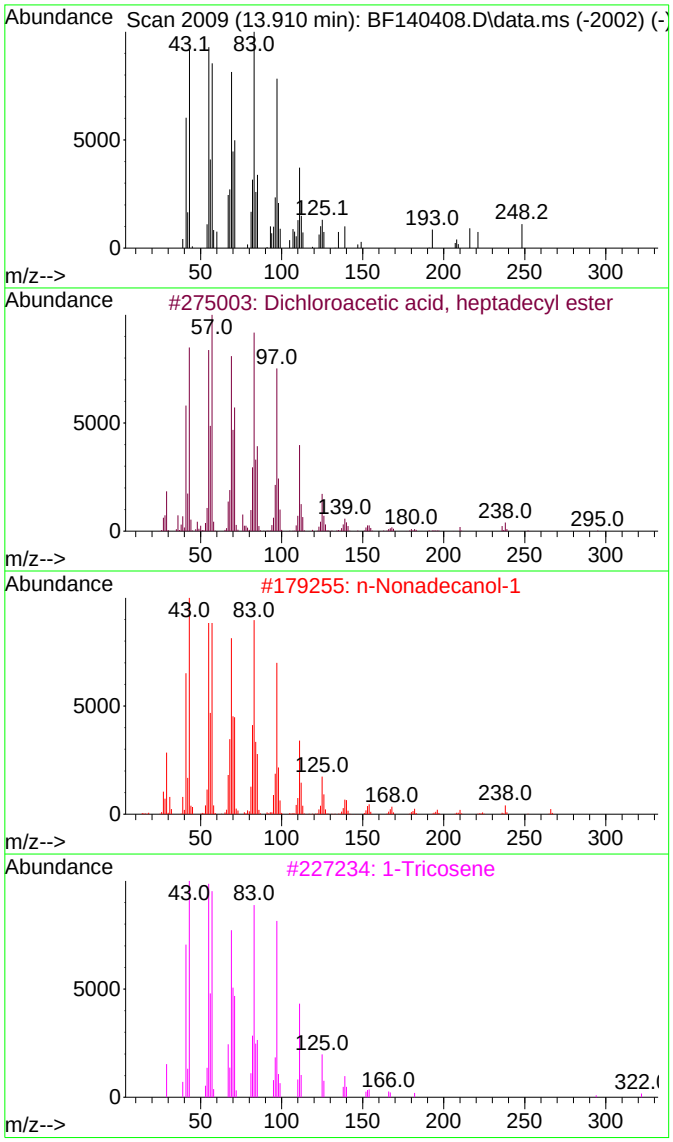
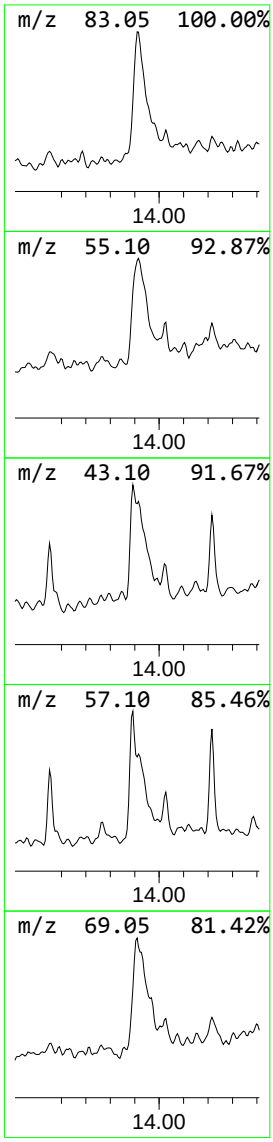
****
Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.19 ng	116853	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	1-Tricosene	322	C23H46	018835-32-0	93
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5	1-Hexadecanol	242	C16H34O	036653-82-4	87





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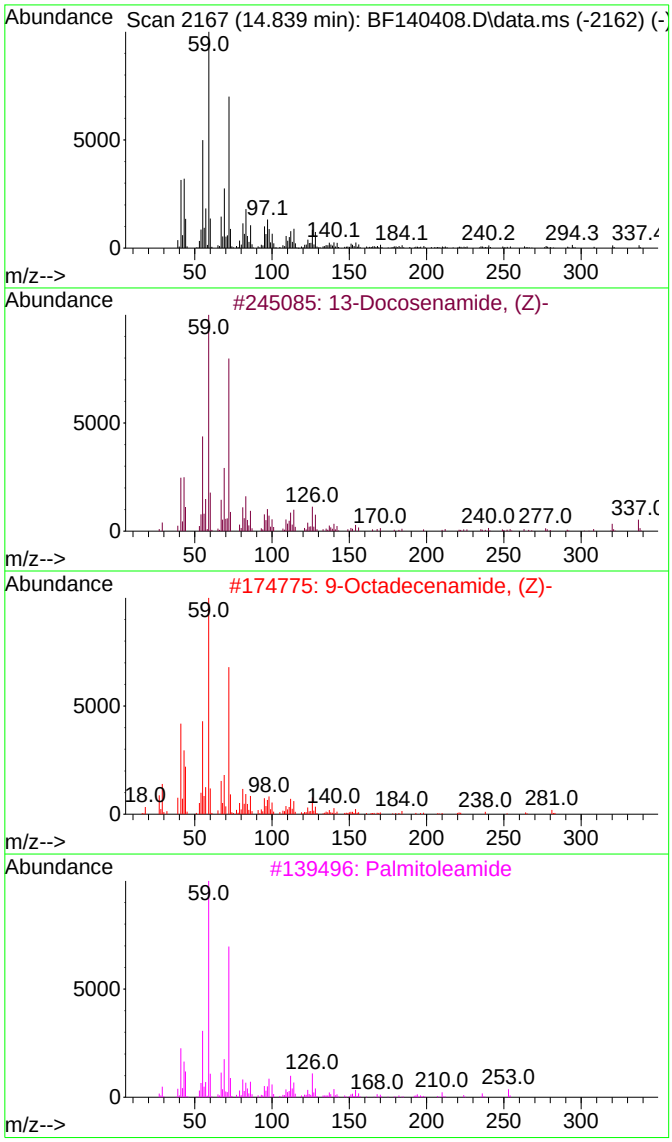
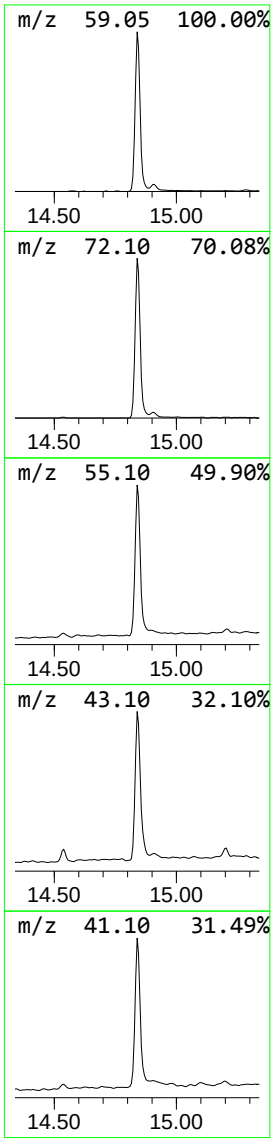
Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	17.51 ng	661126	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	96
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Palmitoleamide	253	C16H31NO	106010-22-4	64
4	7-Nonenamide	155	C9H17NO	090949-53-4	59
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.157	32.1	ng	1244320	1	6.875	774909	20.0
unknown7.510	7.510	2.0	ng	78003	1	6.875	774909	20.0
Benzophenone	10.622	3.1	ng	174698	3	9.910	1113370	20.0
n-Hexadecanoic ...	11.922	4.0	ng	226396	4	11.398	1140280	20.0
Dichloroacetic ...	13.910	3.2	ng	116853	5	14.057	733688	20.0
13-Docosenamide...	14.839	17.5	ng	661126	6	15.574	754961	20.0