LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112224\
Data File : BF140580.D
Acq On : 22 Nov 2024 16:24
Operator : RC/JU
Sample : P4924-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4

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-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	6	15	rVB	617041	868294	40.96%	5.719%
2	5.498	573	579	597	rBV	1177155	1595860	75.28%	10.511%
3	6.504	744	750	772	rBV	1290835	1722499	81.25%	11.345%
4	6.869	807	812	819	rBV	486951	586682	27.67%	3.864%
5	7.428	902	907	918	rBV	830269	1113310	52.51%	7.333%
6	7.686	945	951	964	rBV	16797	32749	1.54%	0.216%
7	8.151	1024	1030	1051	rVB	580732	751408	35.44%	4.949%
8	9.222	1207	1212	1223	rBV	1655624	2120001	100.00%	13.963%
9	9.904	1323	1328	1339	rBV	666249	859963	40.56%	5.664%
10	10.622	1445	1450	1457	rBV	91621	121978	5.75%	0.803%
11	10.698	1457	1463	1479	rBV	884873	1181042	55.71%	7.779%
12	11.398	1576	1582	1591	rBV	598032	804980	37.97%	5.302%
13	11.921	1665	1671	1683	rBV2	122513	226135	10.67%	1.489%
14	12.445	1755	1760	1774	rBV3	27756	78454	3.70%	0.517%
15	12.616	1784	1789	1797	rBV	35571	62265	2.94%	0.410%
16	12.704	1800	1804	1811	rBV6	11332	21219	1.00%	0.140%
17	12.798	1816	1820	1823	rVV2	19383	25361	1.20%	0.167%
18	12.845	1823	1828	1835	rVB	36805	59950	2.83%	0.395%
19	12.980	1846	1851	1860	rVB	1223317	1534214	72.37%	10.105%
20	13.421	1919	1926	1935	rVB2	17776	35682	1.68%	0.235%
21	13.886	1999	2005	2020	rBV3	42023	124637	5.88%	0.821%
22	14.045	2026	2032	2044	rVB	390792	570213	26.90%	3.756%
23	14.804	2157	2161	2168	rBV3	30018	53969	2.55%	0.355%
24	14.898	2172	2177	2181	rVB	89327	126609	5.97%	0.834%
25	15.104	2209	2212	2218	rVB	15567	24251	1.14%	0.160%
26	15.539	2280	2286	2292	rBV	297170	481065	22.69%	3.168%

Sum of corrected areas: 15182790

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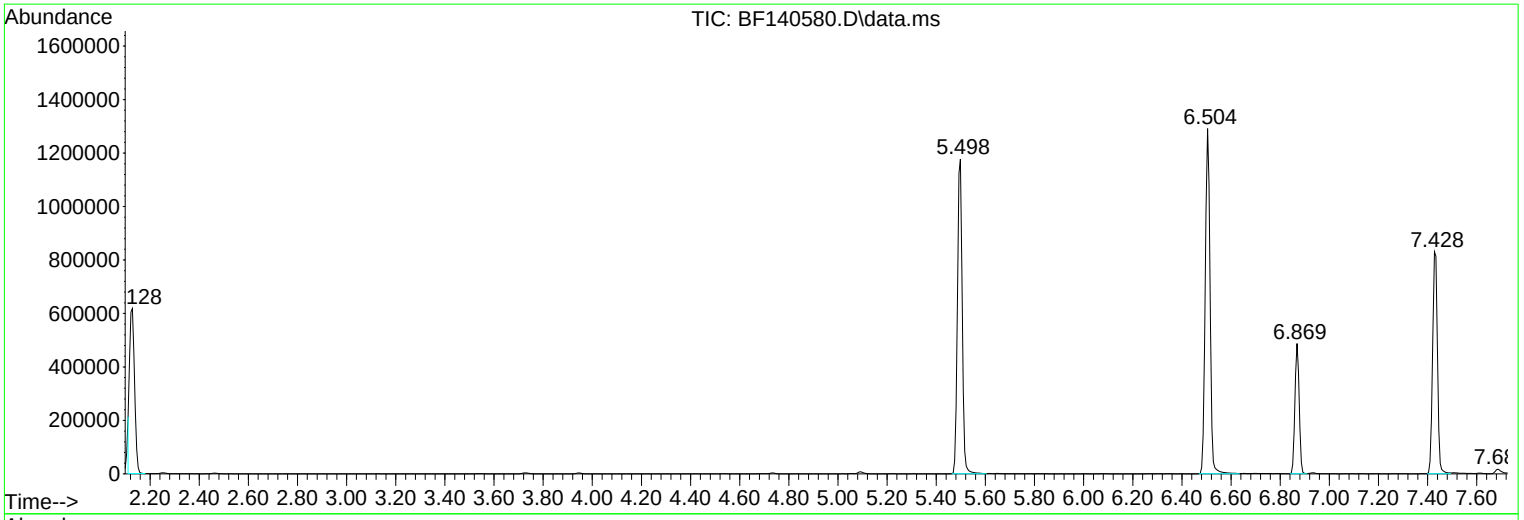
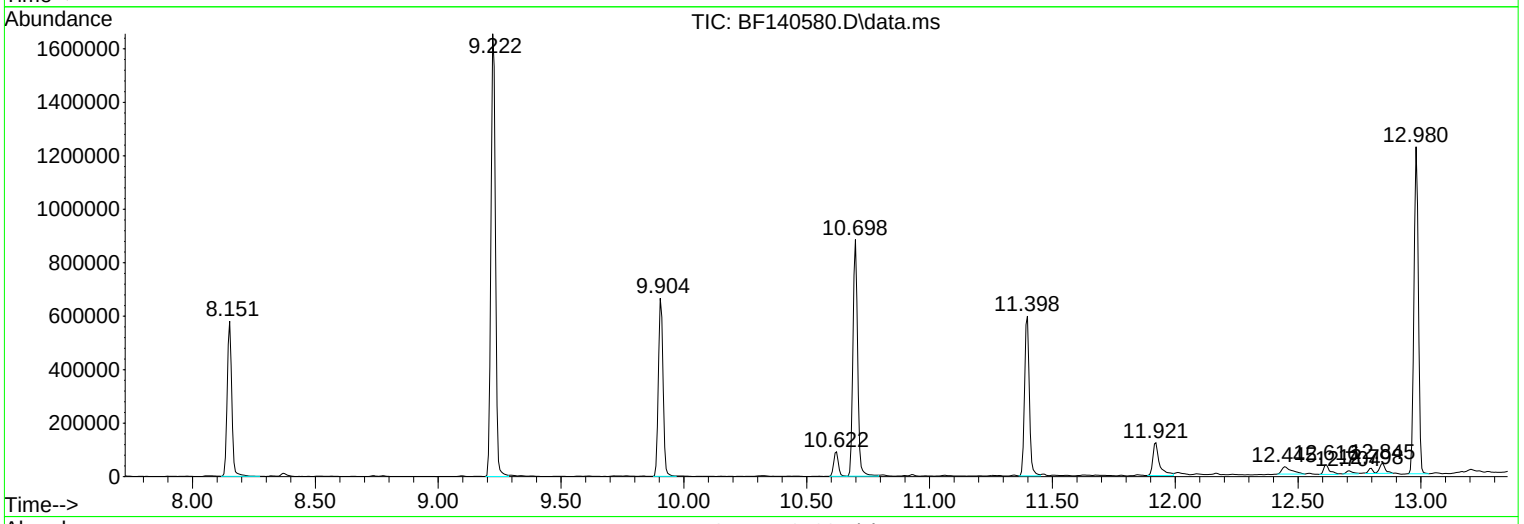
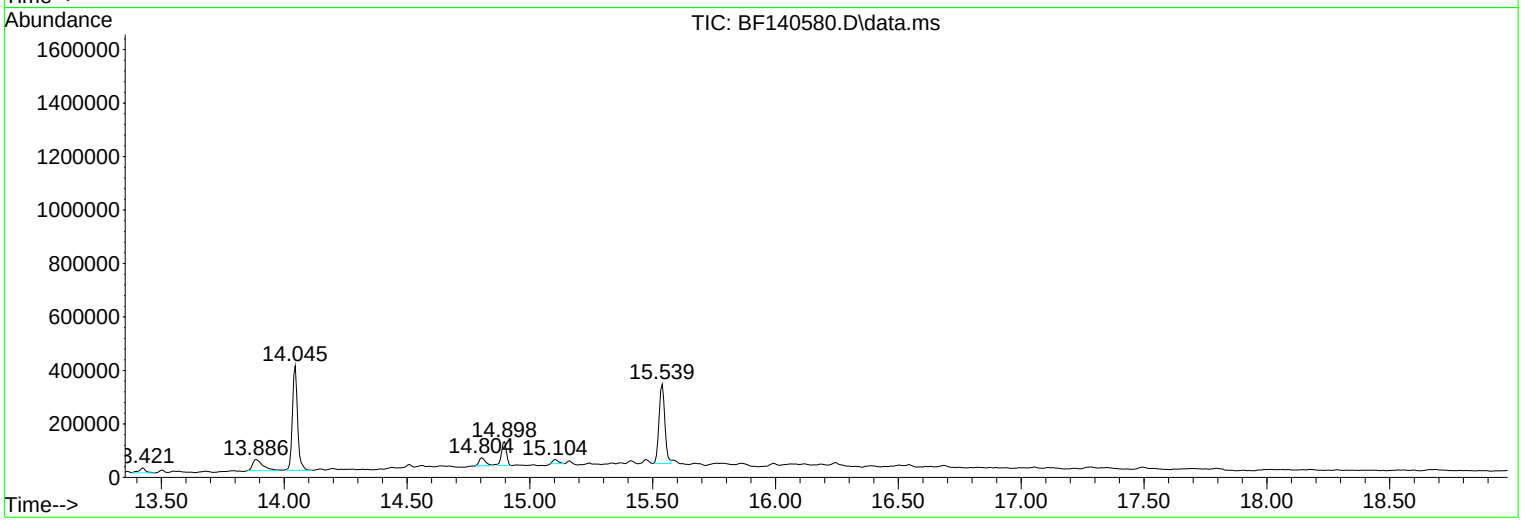
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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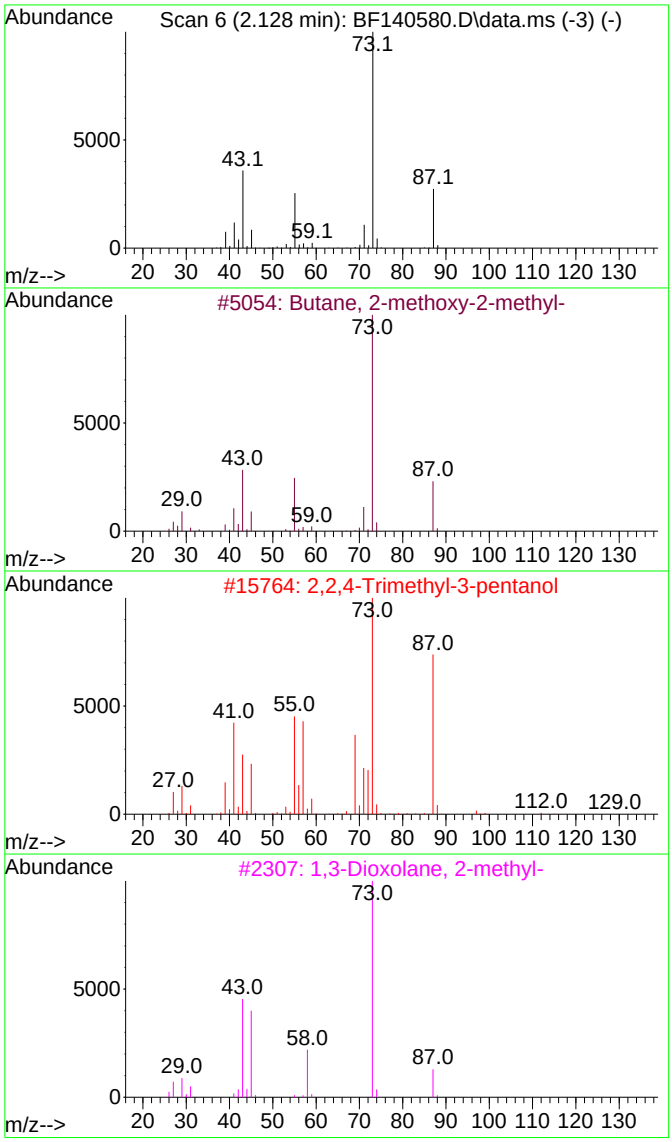
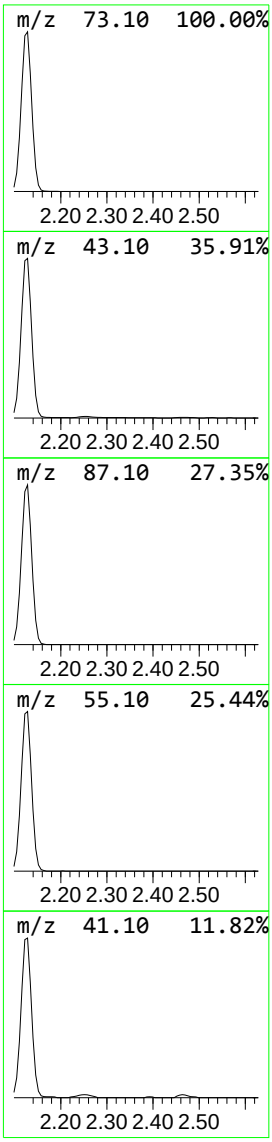
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	29.60 ng	868294	1,4-Dichlorobenzene-d4	6.869

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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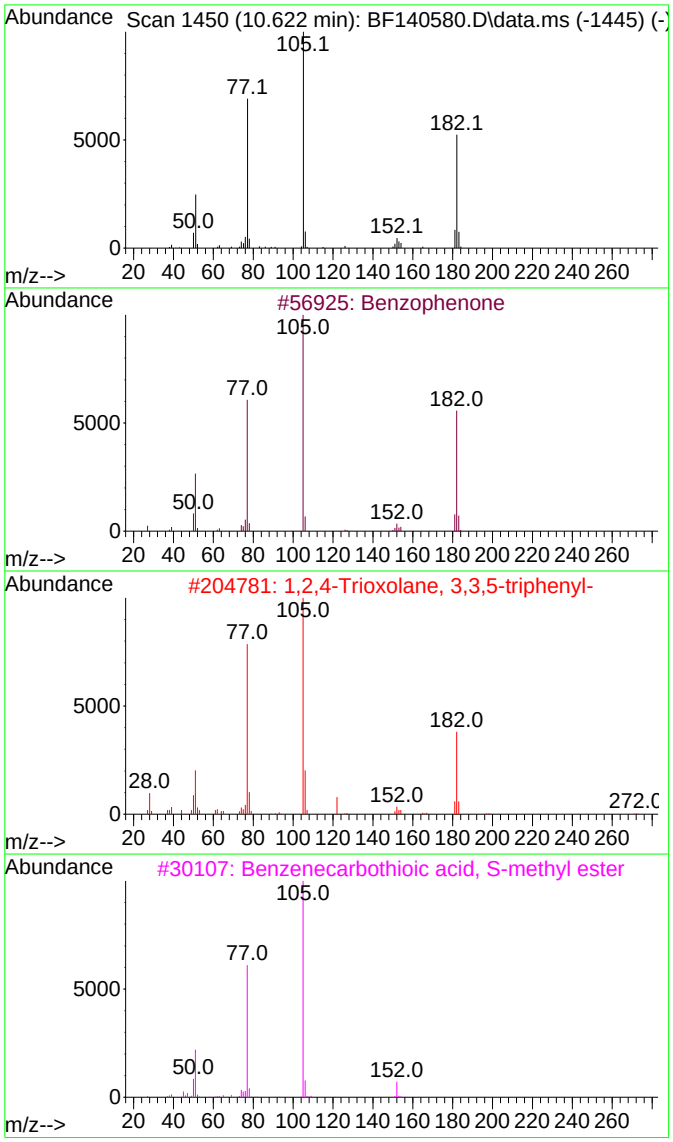
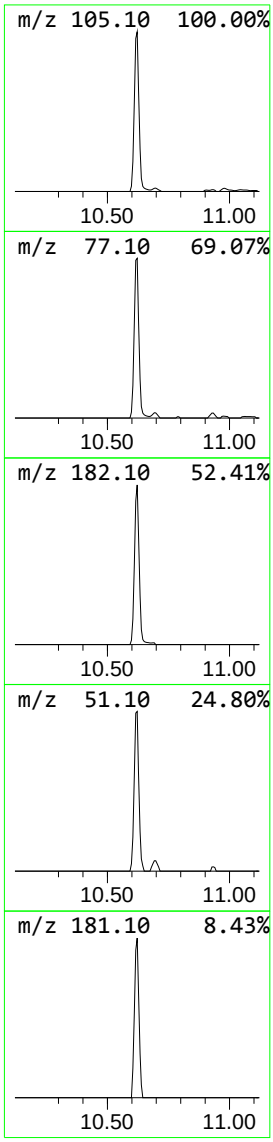
Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	2.84 ng	121978	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47





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Acq On : 22 Nov 2024 16:24
Operator : RC/JU
Sample : P4924-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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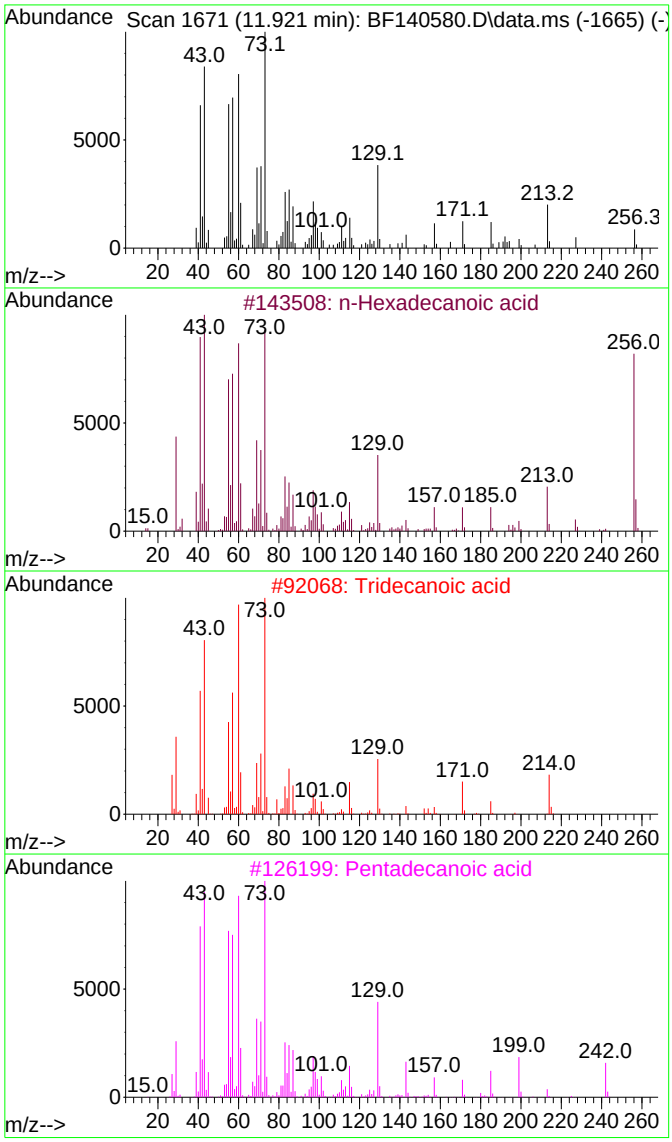
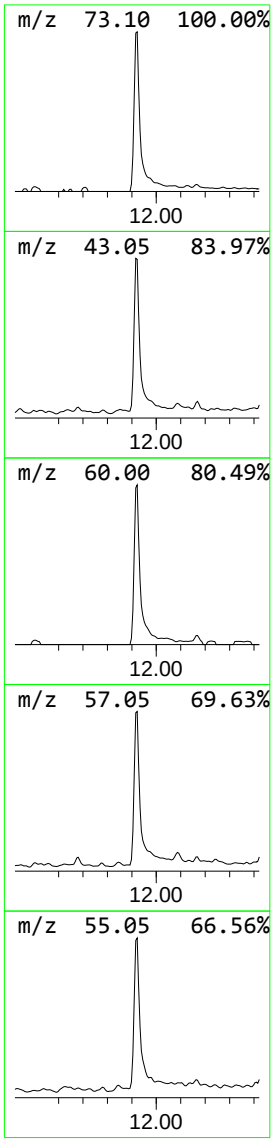
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	5.62 ng	226135	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	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Sample : P4924-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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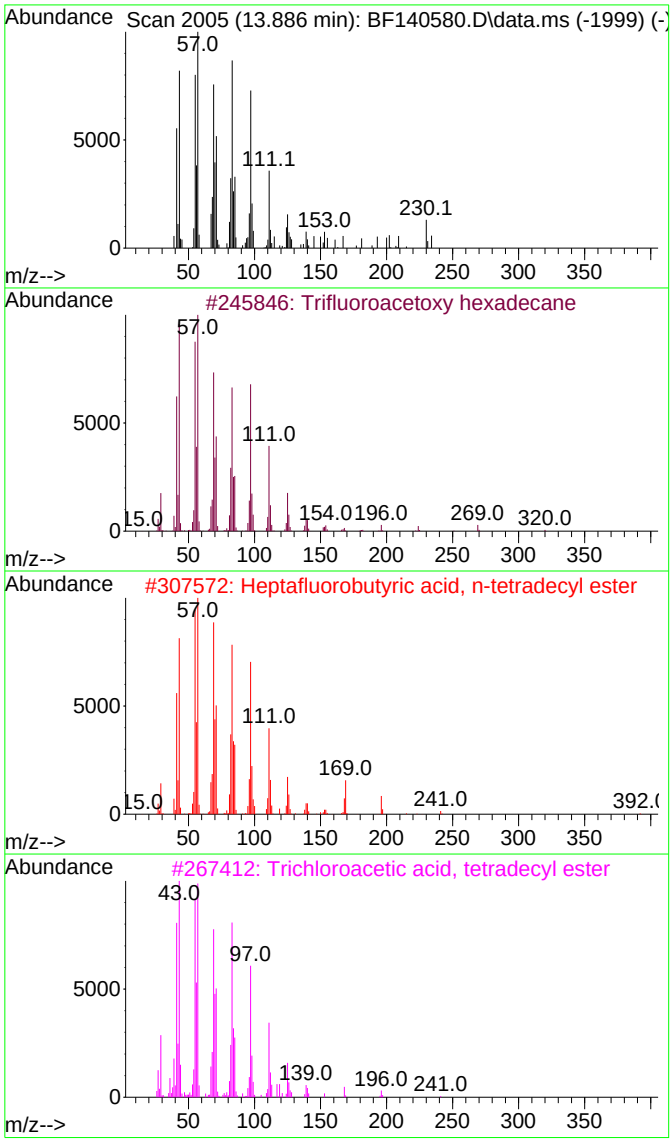
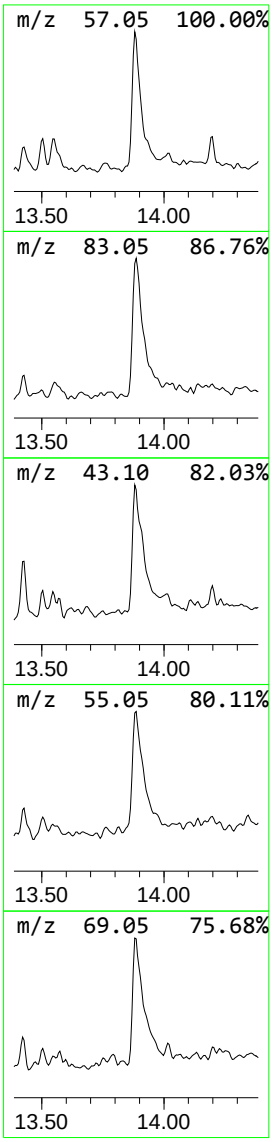
Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.37 ng	124637	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	1-Hexacosene	364	C26H52	018835-33-1	91





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Operator : RC/JU
Sample : P4924-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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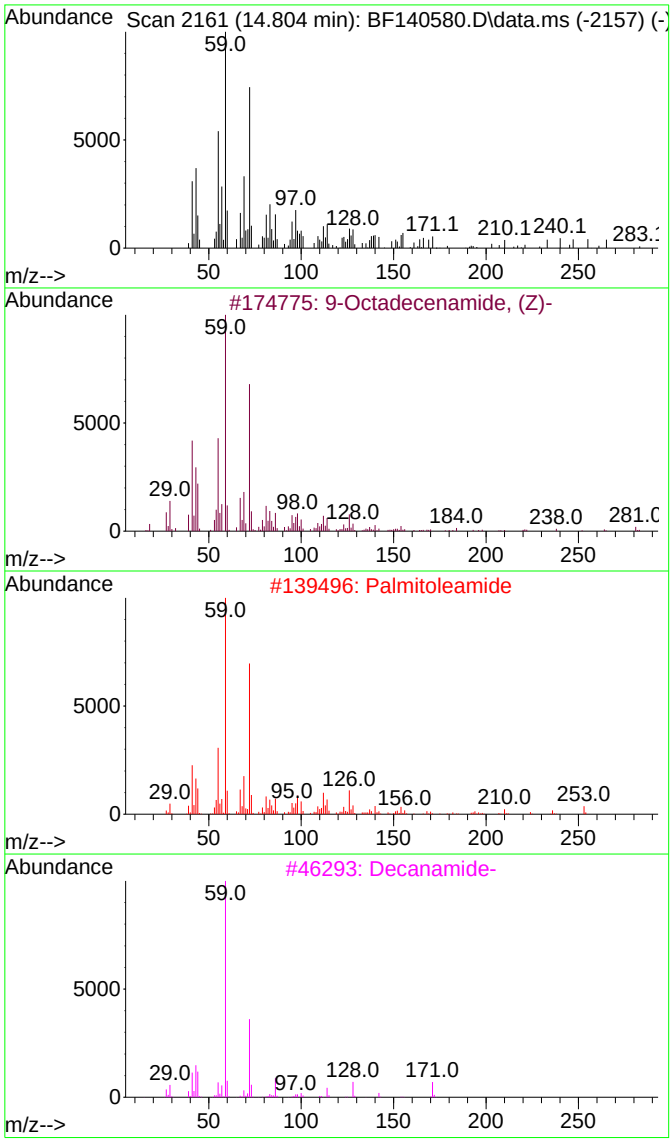
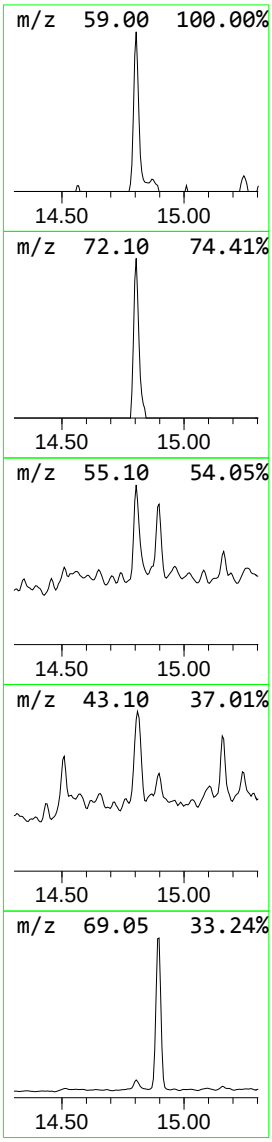
Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.24 ng	53969	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Palmitoleamide	253	C16H31NO	106010-22-4	80
3	Decanamide-	171	C10H21NO	002319-29-1	72
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	68
5	7-Nonenamide	155	C9H17NO	090949-53-4	47





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Sample : P4924-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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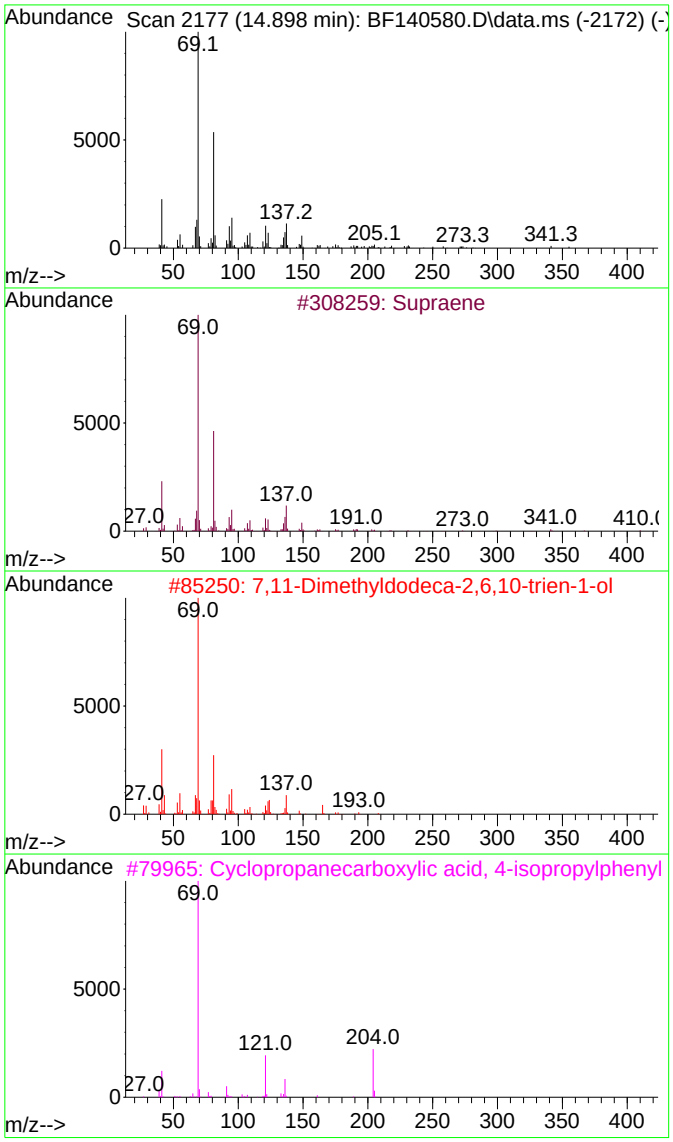
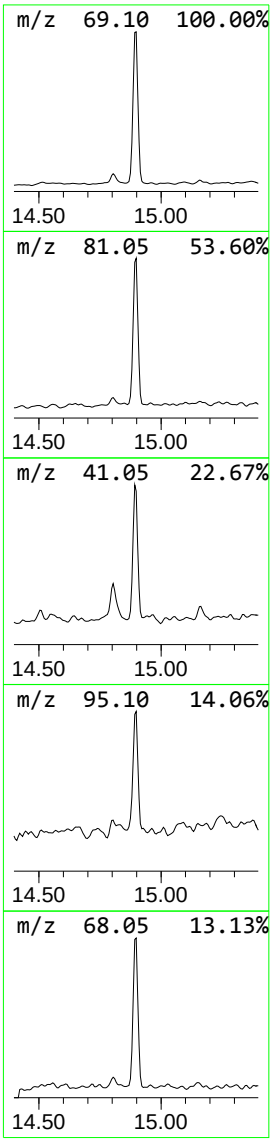
Peak Number 7 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	5.26 ng	126609	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3	Cyclopropanecarboxylic acid, 4-i...	204	C13H16O2	1000331-01-9	52
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52
5	2-Propenoic acid, 2-methyl-, 2-p...	124	C7H8O2	013861-22-8	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112224\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	2.128	29.6	ng	868294	1	6.869	586682	20.0
Benzophenone	10.622	2.8	ng	121978	3	9.904	859963	20.0
n-Hexadecanoic ...	11.922	5.6	ng	226135	4	11.398	804980	20.0
Trifluoroacetox...	13.886	4.4	ng	124637	5	14.045	570213	20.0
9-Octadecenamid...	14.804	2.2	ng	53969	6	15.539	481065	20.0
Supraene	14.898	5.3	ng	126609	6	15.539	481065	20.0