LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
Data File : BF108113.D
Acq On : 13 Aug 2018 13:55
Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.248	491	495	503	rVB	573475	567440	17.68%	1.229%
2	5.637	557	561	565	rBV	2965024	2812827	87.65%	6.094%
3	6.631	726	730	738	rBV	3300277	3148989	98.12%	6.822%
4	6.789	752	757	760	rBV	3331290	3028256	94.36%	6.561%
5	7.019	793	796	800	rVB	1937354	1624508	50.62%	3.519%
6	7.178	819	823	826	rBV	2680057	2197756	68.48%	4.761%
7	7.578	887	891	894	rBV	2289544	1943209	60.55%	4.210%
8	8.307	1011	1015	1018	rBV	2289595	2095646	65.30%	4.540%
9	9.377	1193	1197	1200	rBV	3760054	3209319	100.00%	6.953%
10	9.448	1206	1209	1213	rBV	52137	47815	1.49%	0.104%
11	9.772	1260	1264	1269	rBV	266361	245581	7.65%	0.532%
12	9.977	1296	1299	1303	rVB	92370	73029	2.28%	0.158%
13	10.072	1308	1315	1319	rBV	2699519	2328727	72.56%	5.045%
14	10.483	1381	1385	1388	rVB	121084	104821	3.27%	0.227%
15	10.701	1418	1422	1425	rBV	64958	75456	2.35%	0.163%
16	10.860	1445	1449	1463	rBV	2060393	2043759	63.68%	4.428%
17	10.960	1463	1466	1471	rBV	137783	196535	6.12%	0.426%
18	11.407	1539	1542	1545	rBV	166675	131523	4.10%	0.285%
19	11.436	1545	1547	1550	rVV2	73796	68413	2.13%	0.148%
20	11.571	1566	1570	1572	rBV	2447732	2150262	67.00%	4.659%
21	11.589	1572	1573	1577	rVB	351185	280058	8.73%	0.607%
22	11.642	1580	1582	1586	rVB	94796	77622	2.42%	0.168%
23	11.795	1605	1608	1610	rBV3	48961	47593	1.48%	0.103%
24	11.836	1613	1615	1618	rVV	147620	108964	3.40%	0.236%
25	11.936	1629	1632	1636	rVB	733067	592564	18.46%	1.284%
26	12.071	1650	1655	1658	rBV	419038	430090	13.40%	0.932%
27	12.101	1658	1660	1664	rVB2	96547	86171	2.69%	0.187%
28	12.189	1671	1675	1677	rBV2	82036	89246	2.78%	0.193%
29	12.248	1682	1685	1687	rVB	119080	95566	2.98%	0.207%
30	12.395	1708	1710	1713	rVB3	49010	45352	1.41%	0.098%
31	12.630	1746	1750	1752	rBV	2121198	1961572	61.12%	4.250%
32	12.654	1752	1754	1761	rVB	2091574	1794050	55.90%	3.887%
33	12.736	1761	1768	1774	rBV	526818	610884	19.03%	1.323%
34	12.789	1774	1777	1781	rVB	712142	584886	18.22%	1.267%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.024	1811	1817	1822	rVB	578132	688829	21.46%	1.492%
36	13.154	1835	1839	1843	rBV	2656475	2599104	80.99%	5.631%
37	13.301	1862	1864	1866	rBV3	55314	56887	1.77%	0.123%
38	13.460	1886	1891	1895	rBV3	126792	227762	7.10%	0.493%
39	13.577	1909	1911	1914	rBV3	105162	104996	3.27%	0.227%
40	13.665	1921	1926	1933	rVB	635792	960664	29.93%	2.081%
41	14.071	1992	1995	1999	rBV4	109720	135888	4.23%	0.294%
42	14.148	2004	2008	2012	rBV	251984	357580	11.14%	0.775%
43	14.230	2017	2022	2025	rVV2	2058135	2151361	67.03%	4.661%
44	14.254	2025	2026	2033	rVB	269964	248373	7.74%	0.538%
45	14.677	2095	2098	2104	rVB	301433	398037	12.40%	0.862%
46	15.101	2167	2170	2174	rVB	444591	473703	14.76%	1.026%
47	15.336	2207	2210	2213	rBV	220310	298323	9.30%	0.646%
48	15.742	2276	2279	2285	rVB	209149	292317	9.11%	0.633%
49	15.818	2286	2292	2305	rVB	1388258	2265130	70.58%	4.907%

Sum of corrected areas: 46157443

LSC Report - Integrated Chromatogram

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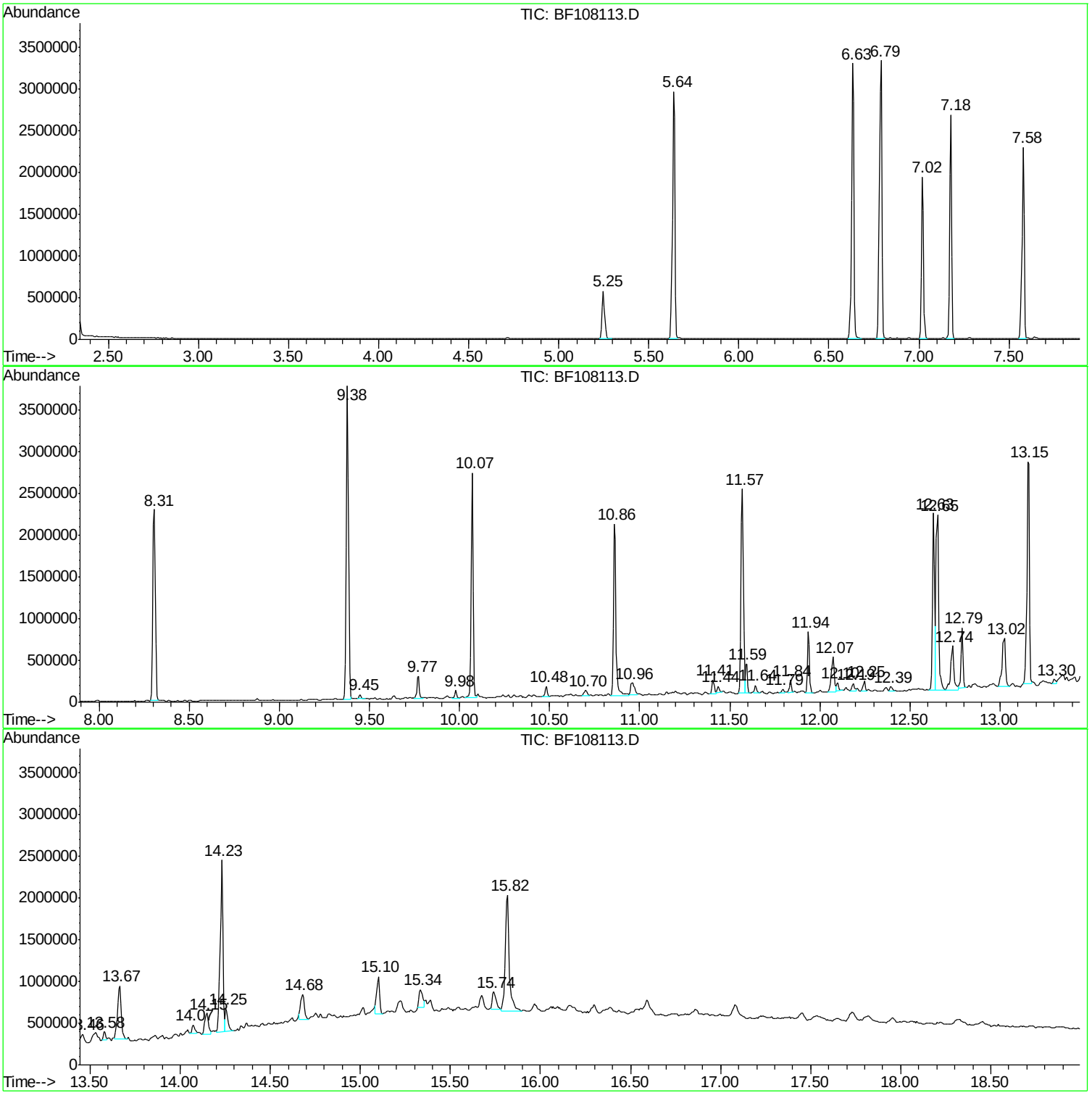
Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
Data File : BF108113.D
Acq On : 13 Aug 2018 13:55
Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

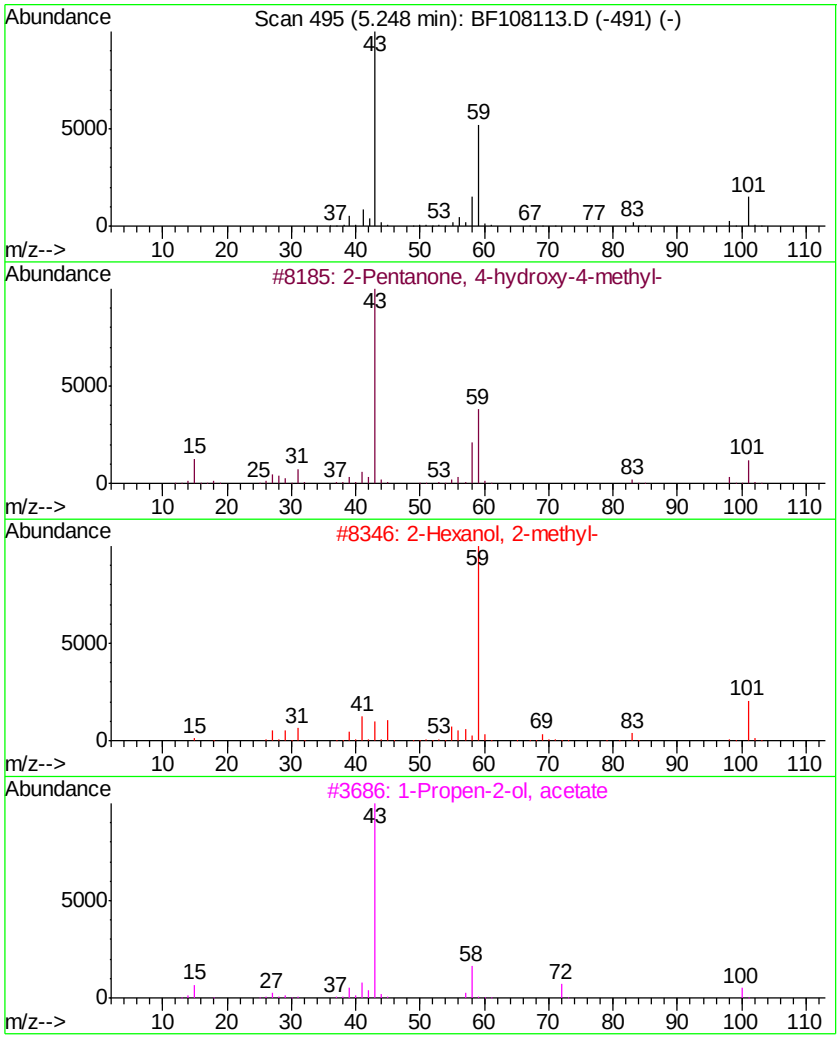
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

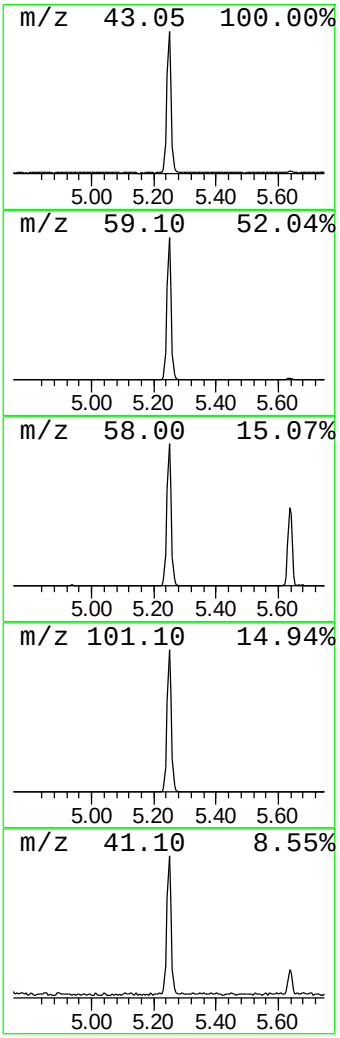
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	6.99 ng	567440	1,4-Dichlorobenzene-d4	7.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Allyl acetate	100	C5H8O2	000591-87-7	9





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Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

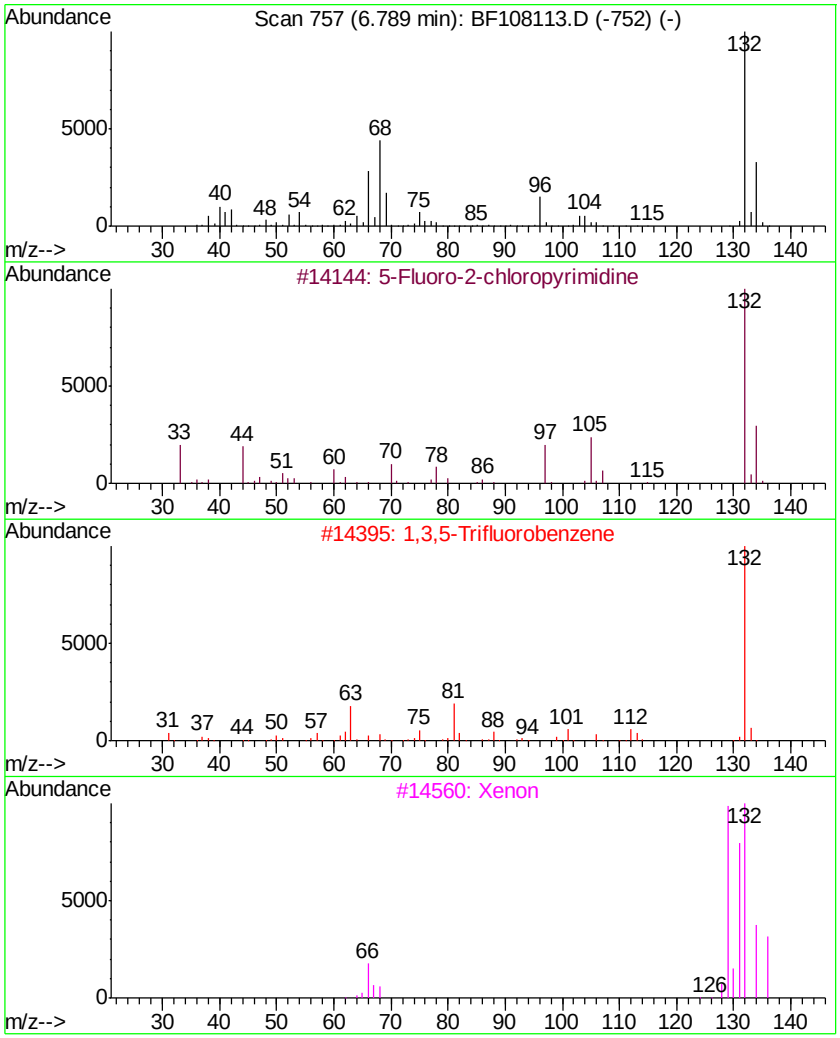
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

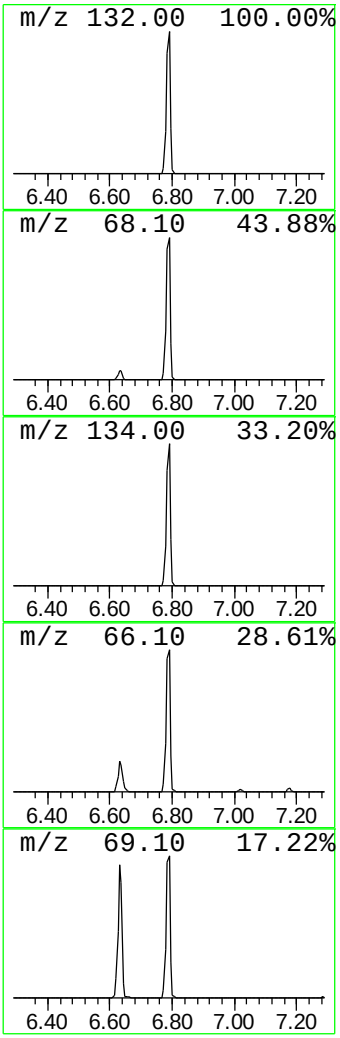
****

Peak Number 2 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	37.28 ng	3028260	1,4-Dichlorobenzene-d4	7.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	Xenon	132	Xe	007440-63-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Misc :
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Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

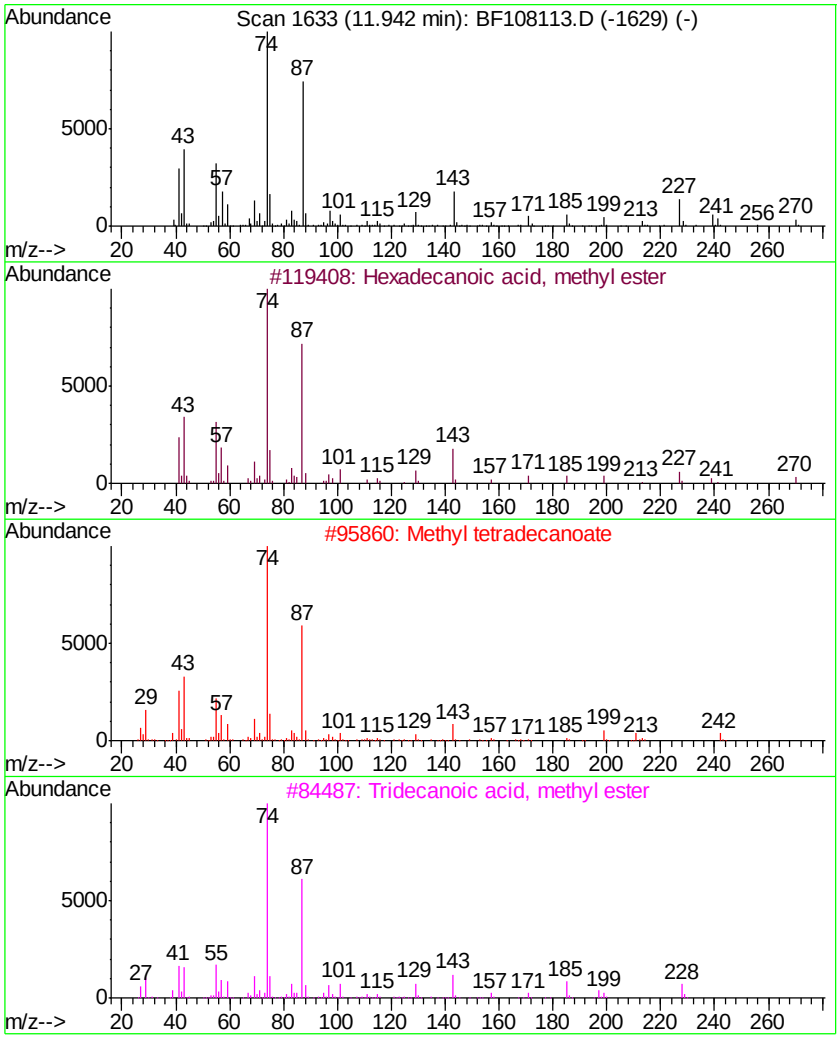
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

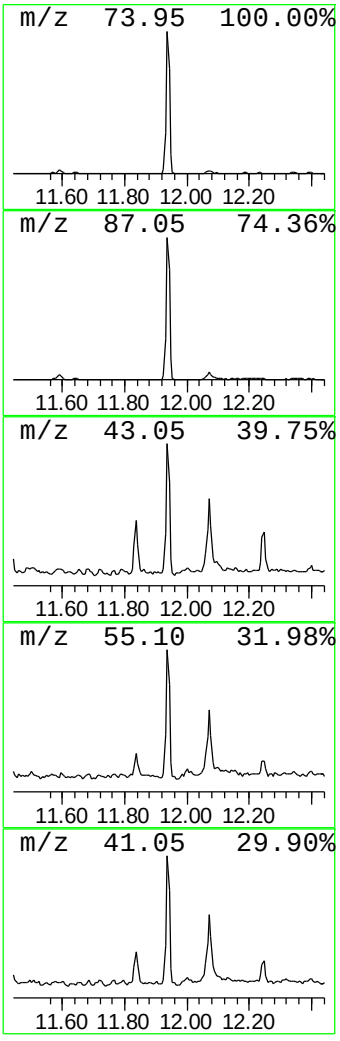
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	5.51 ng	592564	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





Library Search Compound Report

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Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

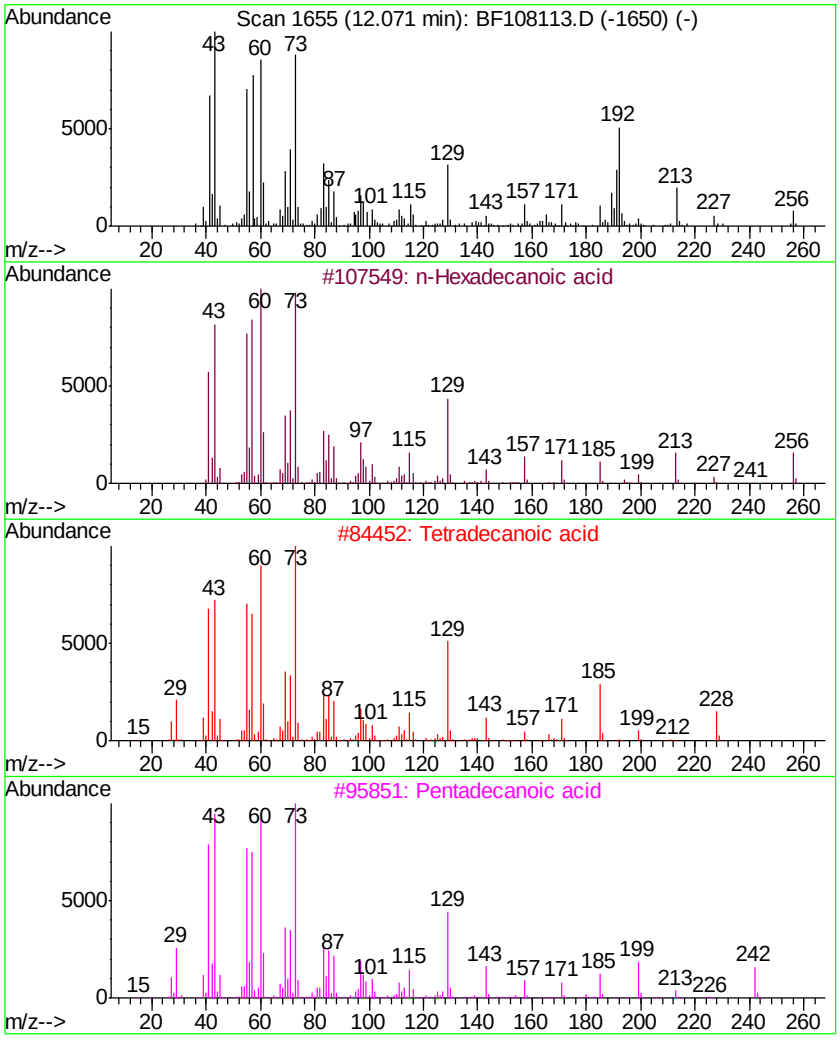
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

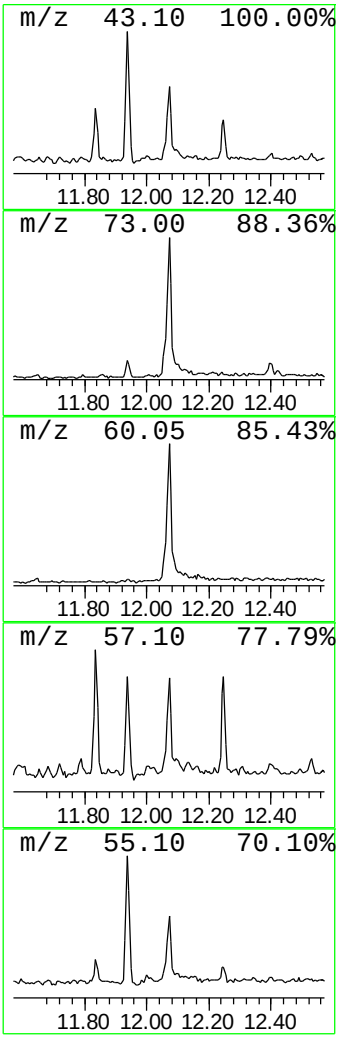
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	4.00 ng	430090	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	55





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Misc :
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Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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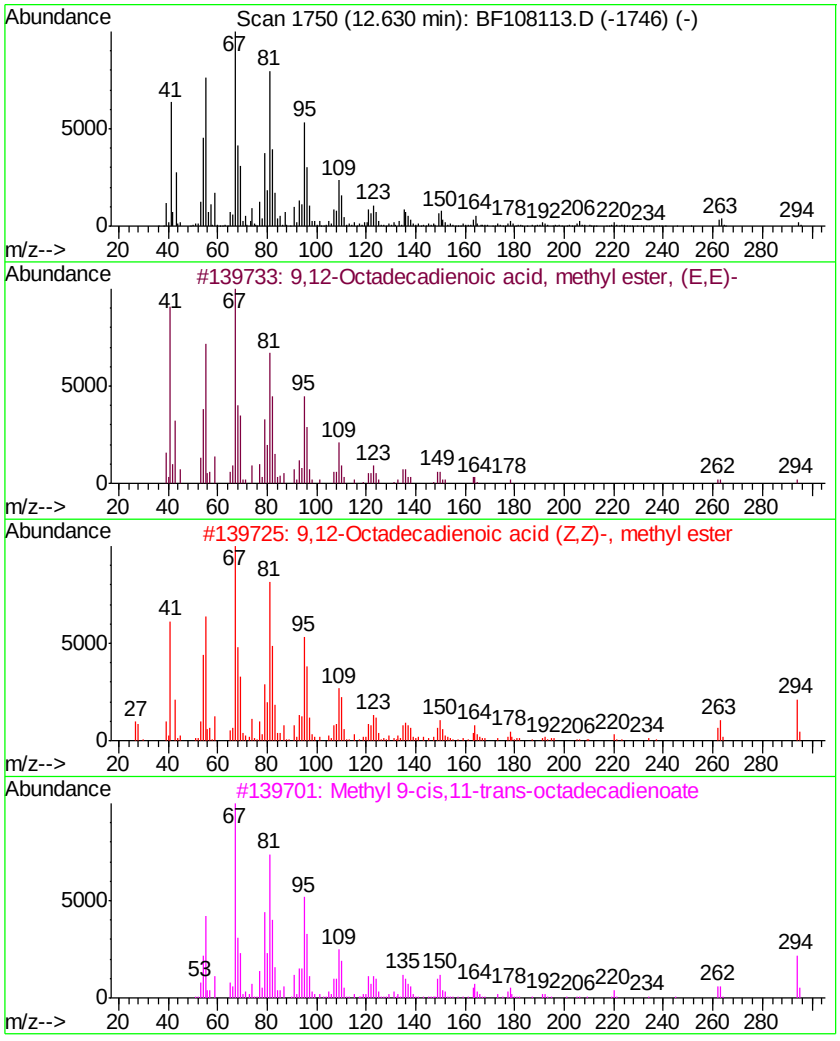
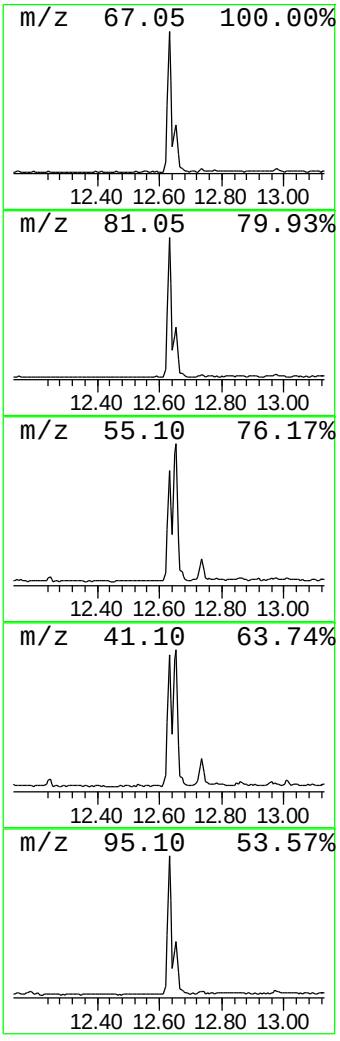
****

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	18.25 ng	1961570	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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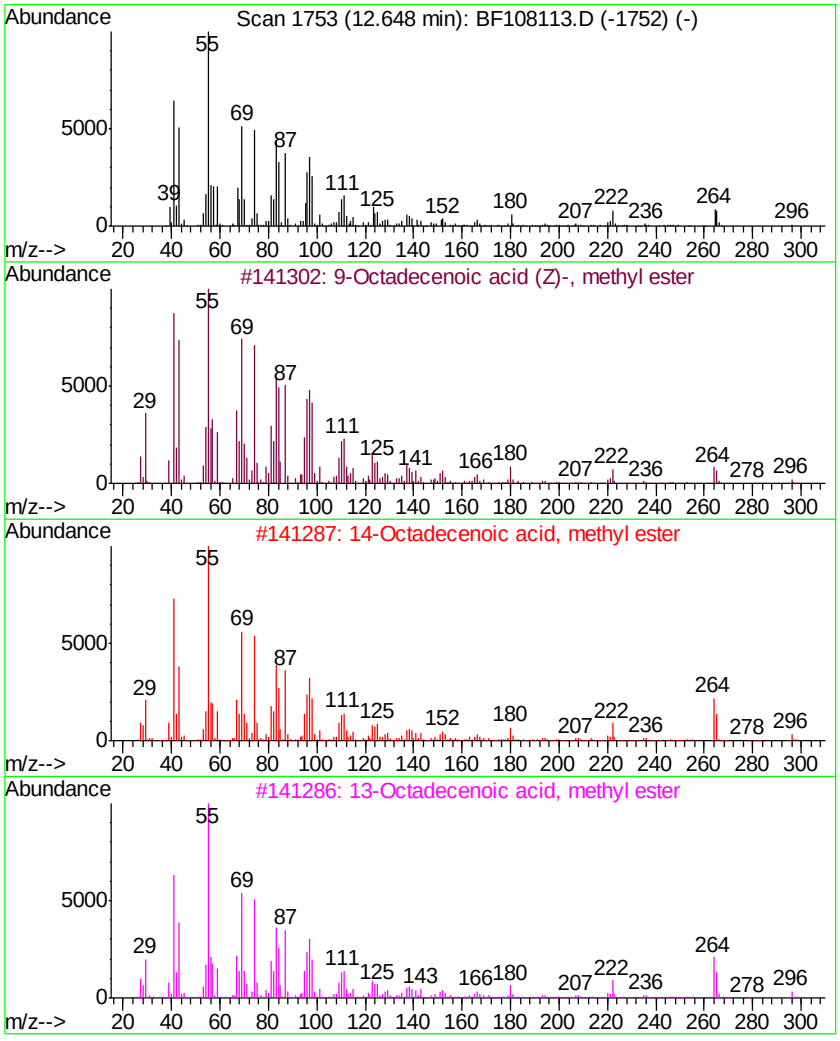
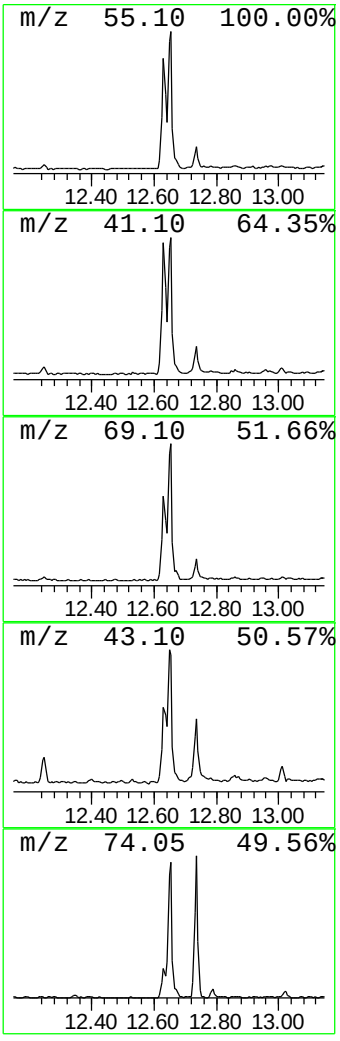
Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	16.69 ng	1794050	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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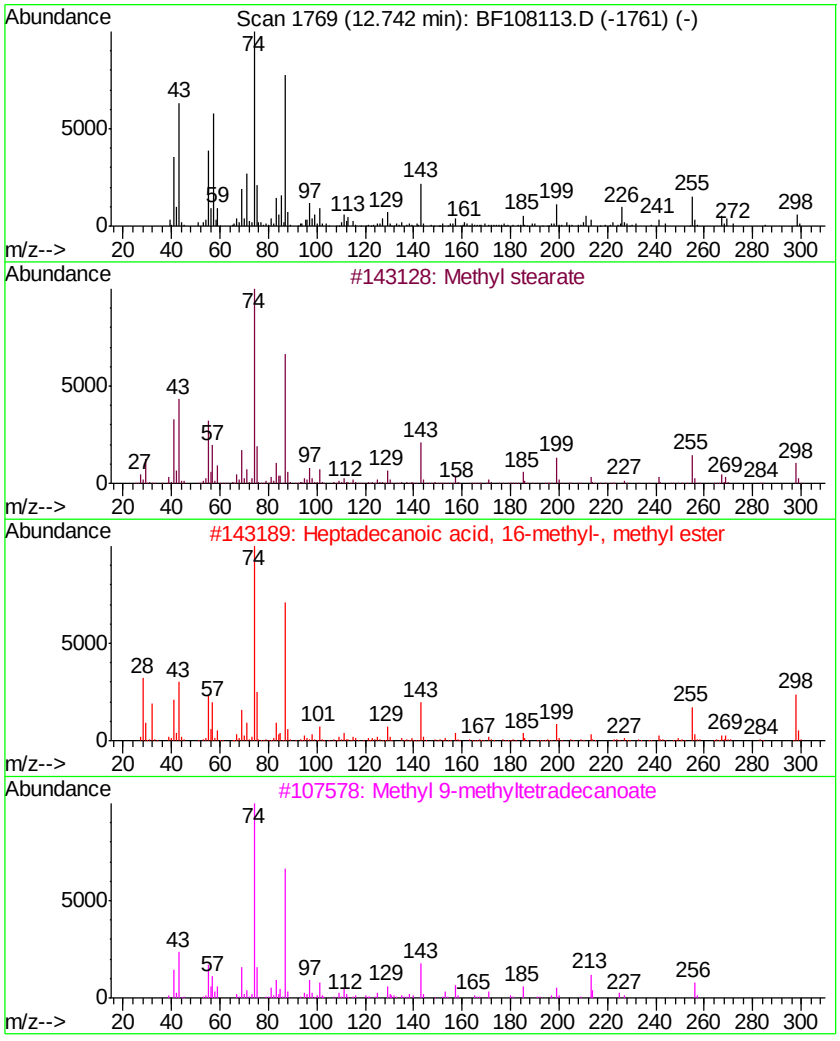
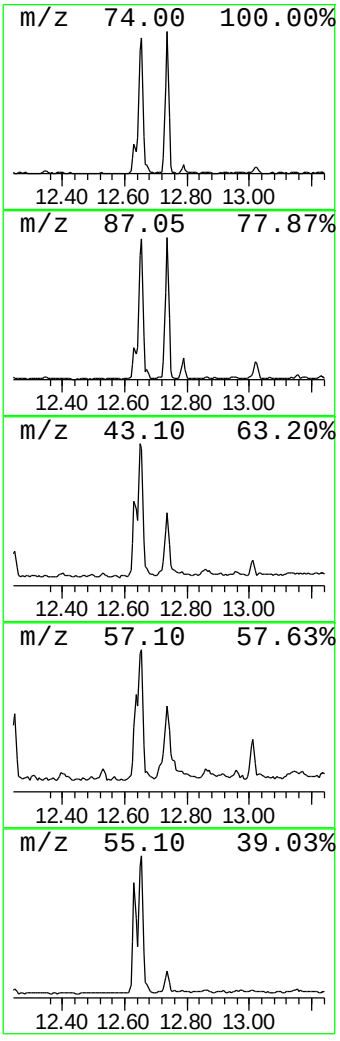
Peak Number 8 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	5.68 ng	610884	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	96
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
3	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	86





Library Search Compound Report

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Acq On : 13 Aug 2018 13:55
Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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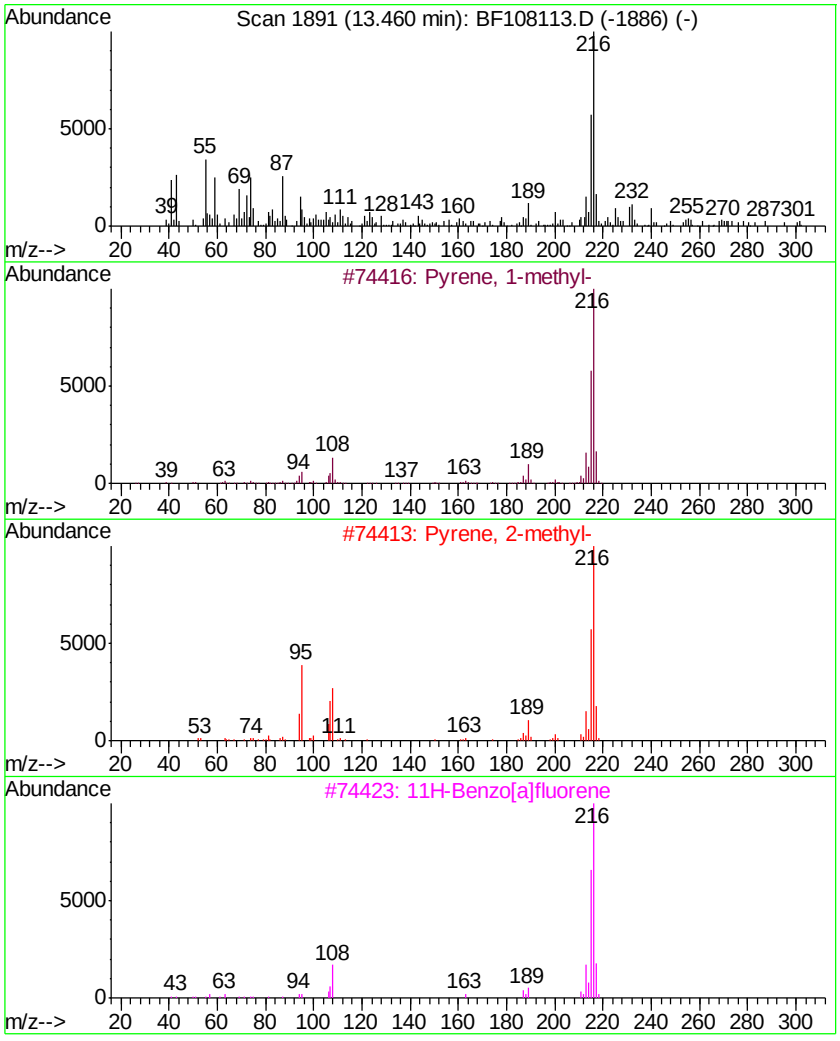
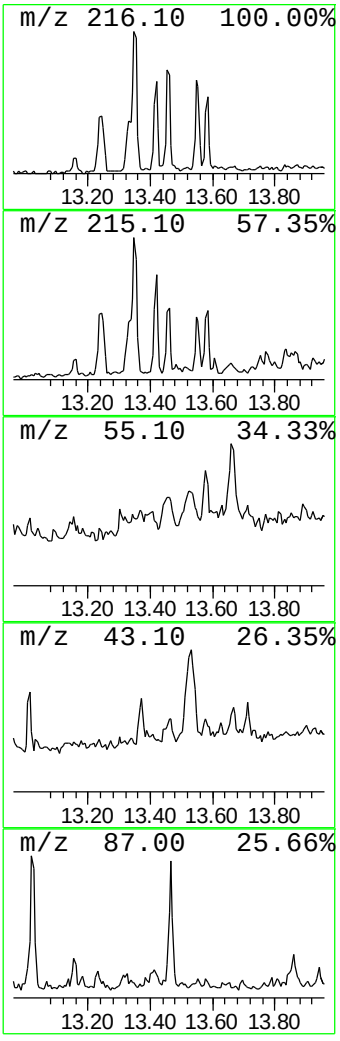
****

Peak Number 9 Pyrene, 1-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	2.12 ng	227762	Chrysene-d12	14.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	95
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	78
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	60
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	53
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
Data File : BF108113.D
Acq On : 13 Aug 2018 13:55
Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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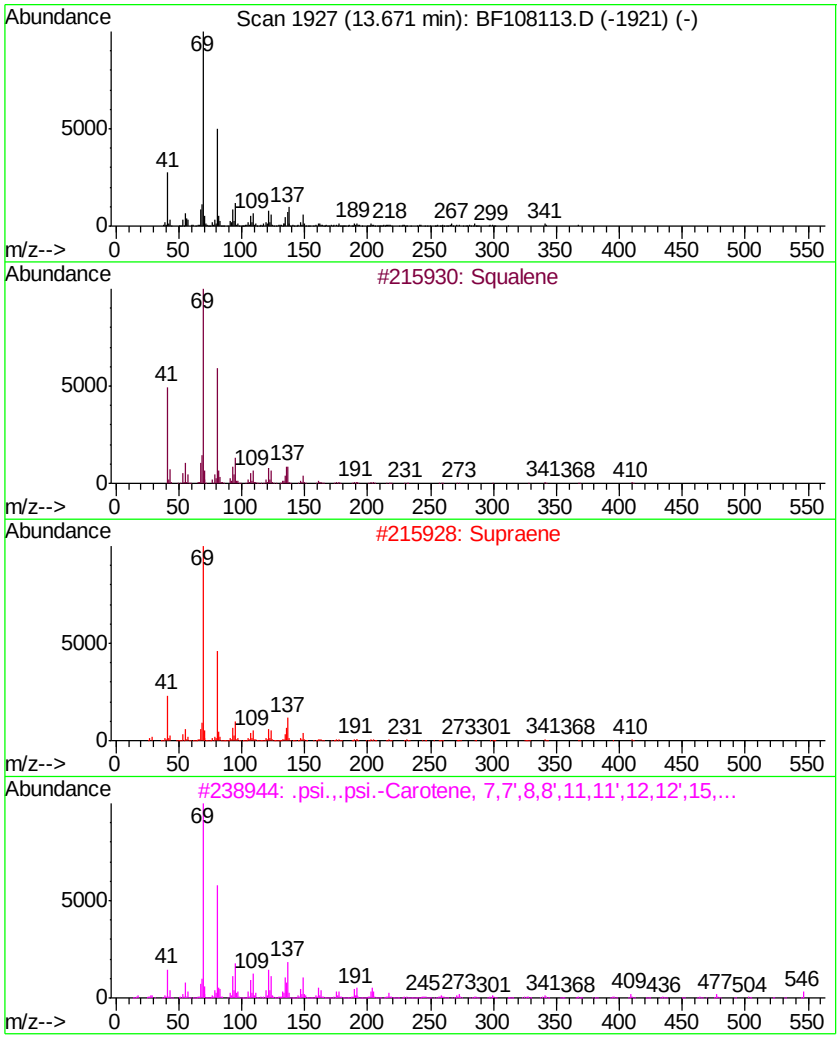
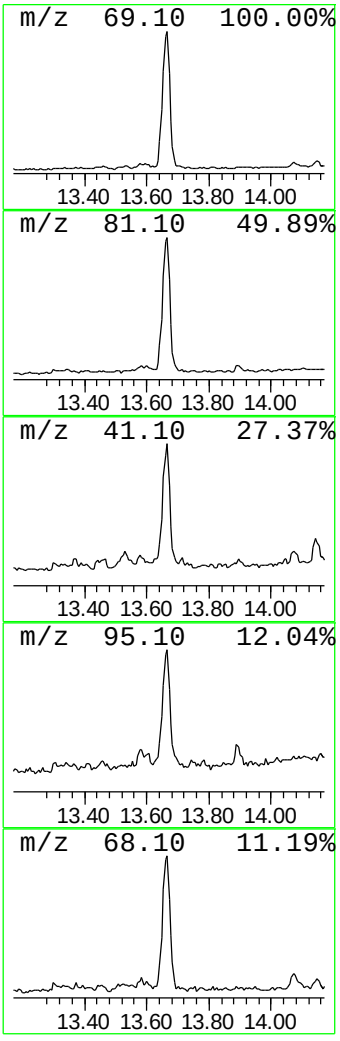
Peak Number 10 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	8.93 ng	960664	Chrysene-d12	14.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	53
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
Data File : BF108113.D
Acq On : 13 Aug 2018 13:55
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
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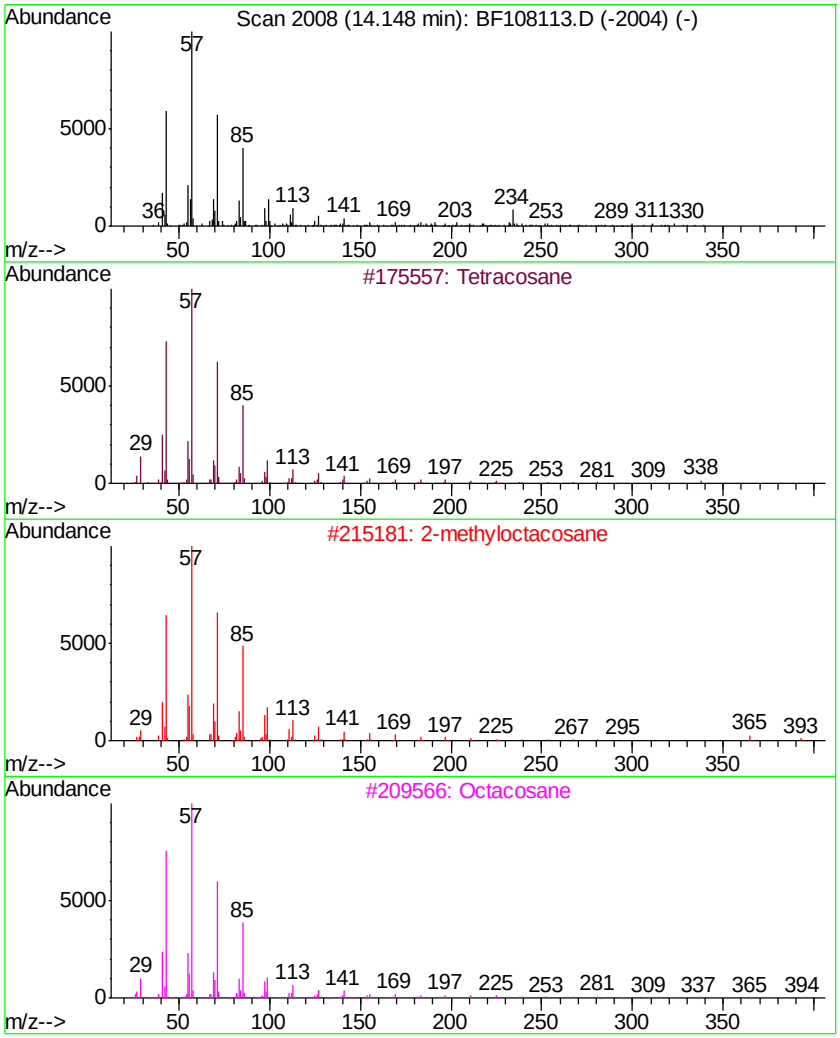
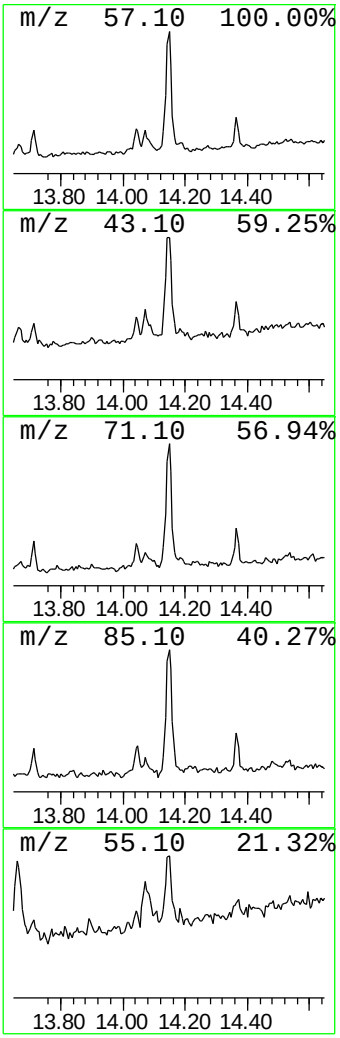
Peak Number 11 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.15	3.32 ng	357580	Chrysene-d12	14.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87





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Data File : BF108113.D
Acq On : 13 Aug 2018 13:55
Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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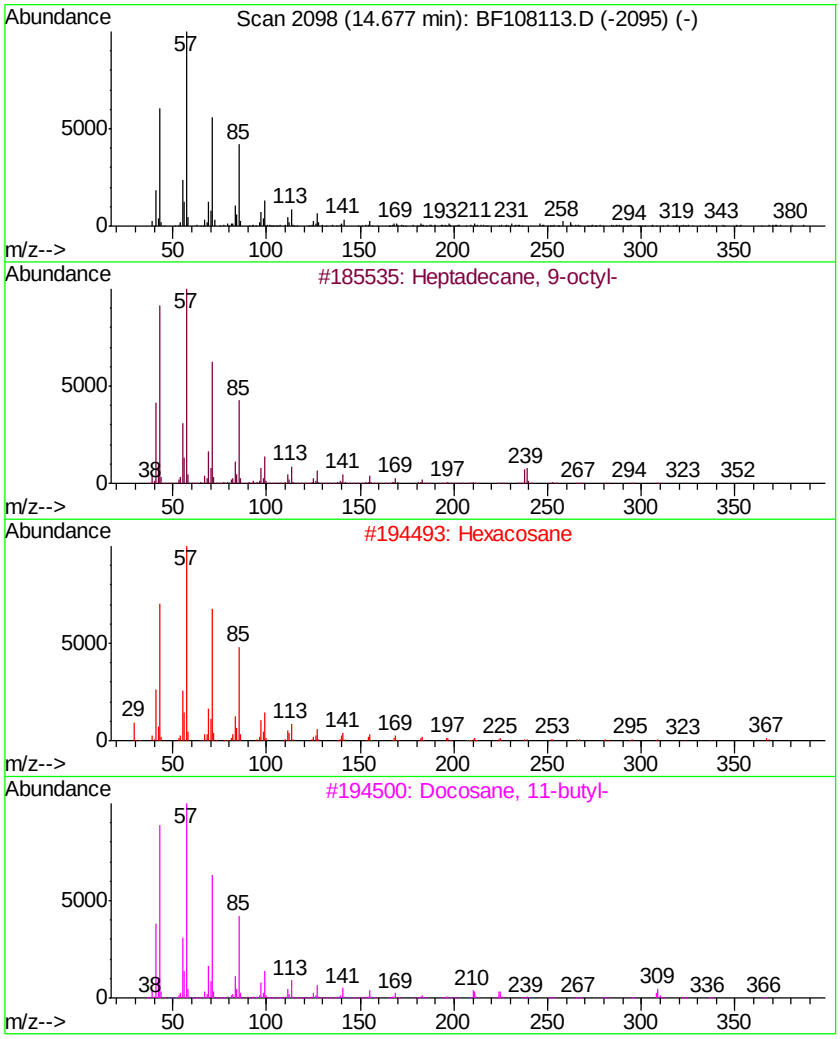
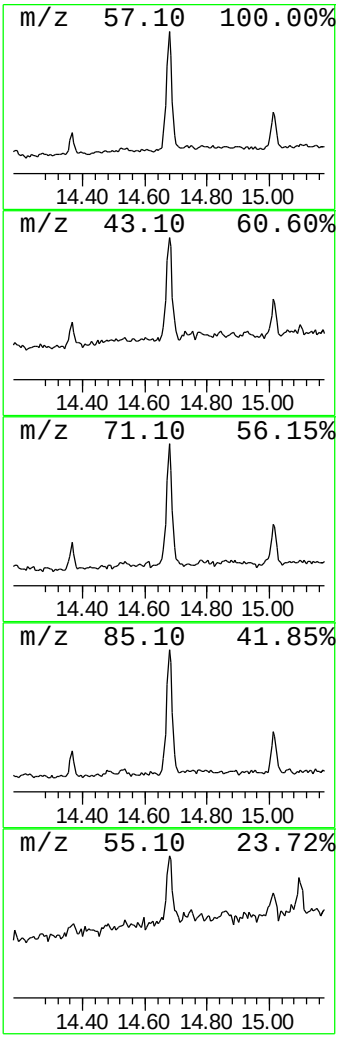
Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	3.70 ng	398037	Chrysene-d12	14.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2	Hexacosane	366	C26H54	000630-01-3	90
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Pentadecane	212	C15H32	000629-62-9	87





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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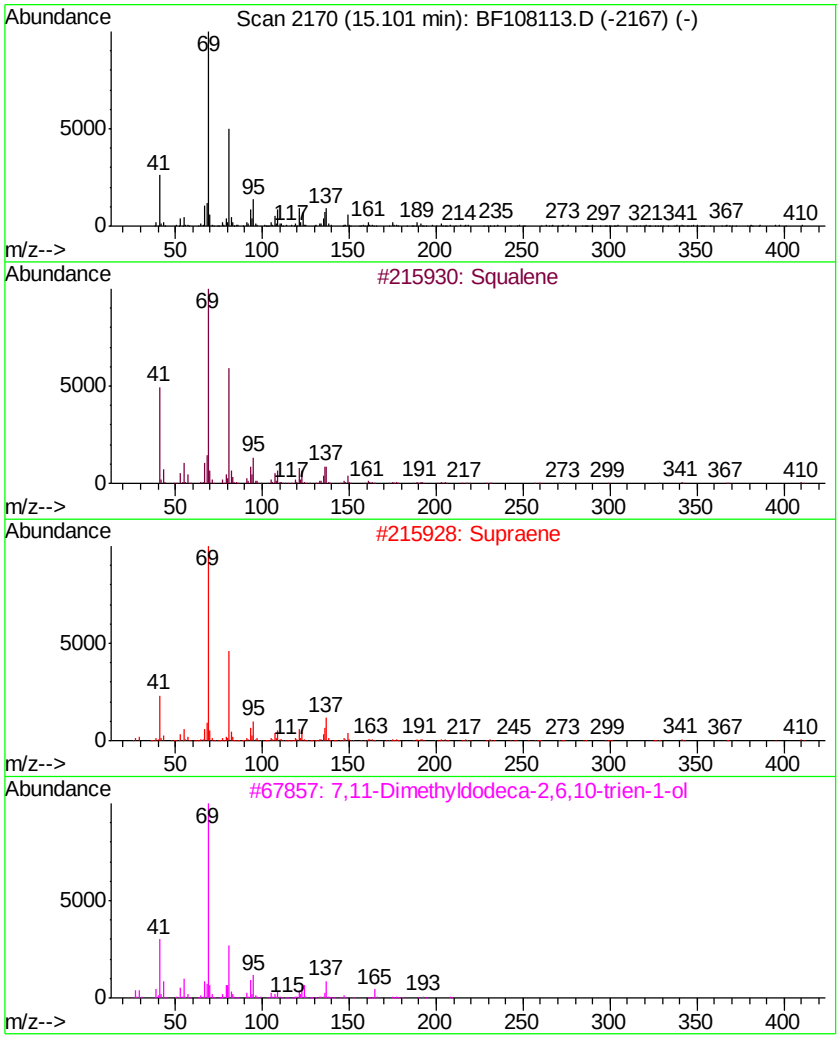
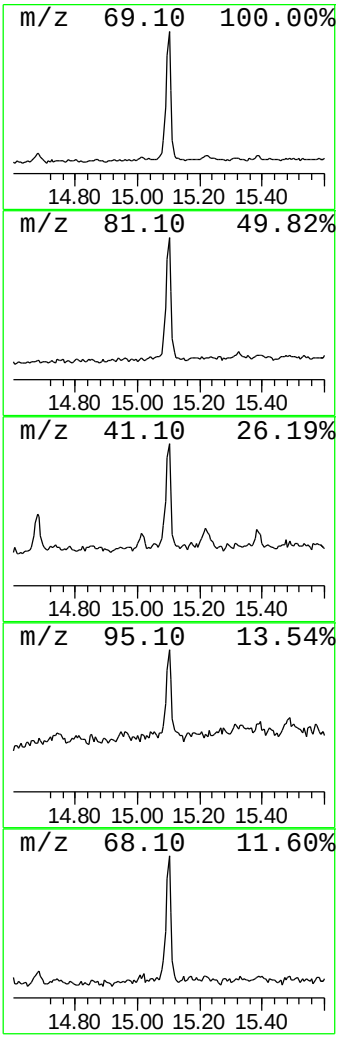
Peak Number 13 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	4.18 ng	473703	Perylene-d12	15.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	98
2	Supraene	410	C30H50	007683-64-9	94
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4	(Z)-all-trans-3,7,11-Trimethyl-2...	235	C15H25NO	123257-83-0	59
5	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	59





Tentatively Identified Compound (LSC) summary

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Data File : BF108113.D
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Operator : JU/SJ
Sample : J4272-11 2X
Misc :
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Instrument : BNA_F
ClientSampleId : JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.25	7.0	ng	567440	1	7.02	1624510	20.0
unknown6.79	6.79	37.3	ng	3028260	1	7.02	1624510	20.0
Hexadecanoic acid...	11.94	5.5	ng	592564	4	11.57	2150260	20.0
n-Hexadecanoic acid	12.07	4.0	ng	430090	4	11.57	2150260	20.0
9,12-Octadecadien...	12.63	18.3	ng	1961570	4	11.57	2150260	20.0
9-Octadecenoic ac...	12.65	16.7	ng	1794050	4	11.57	2150260	20.0
Methyl stearate	12.74	5.7	ng	610884	4	11.57	2150260	20.0
Pyrene, 1-methyl-	13.46	2.1	ng	227762	5	14.23	2151360	20.0
Supraene	13.67	8.9	ng	960664	5	14.23	2151360	20.0
Tetracosane	14.15	3.3	ng	357580	5	14.23	2151360	20.0
Heptadecane, 9-oc...	14.68	3.7	ng	398037	5	14.23	2151360	20.0
Squalene	15.10	4.2	ng	473703	6	15.82	2265130	20.0