LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
Data File : BF108115.D
Acq On : 13 Aug 2018 14:49
Operator : JU/SJ
Sample : J4272-15 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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	504	rVB	579112	606739	17.54%	1.232%
2	5.642	557	562	565	rBV	3318552	2939989	85.01%	5.969%
3	6.636	726	731	740	rBV	3486425	3192790	92.32%	6.482%
4	6.789	753	757	760	rBV	3657305	3095391	89.51%	6.284%
5	6.842	763	766	770	rVB	70551	61433	1.78%	0.125%
6	7.025	793	797	800	rBV	1976060	1767704	51.12%	3.589%
7	7.178	819	823	826	rBV	2947267	2390732	69.13%	4.854%
8	7.578	887	891	894	rBV	2162381	1972499	57.04%	4.005%
9	8.307	1011	1015	1018	rBV	2612115	2182574	63.11%	4.431%
10	8.583	1057	1062	1068	rBV9	28233	58435	1.69%	0.119%
11	8.877	1110	1112	1117	rVB3	36109	42540	1.23%	0.086%
12	9.125	1151	1154	1159	rVB5	32528	37143	1.07%	0.075%
13	9.242	1171	1174	1178	rBV4	30037	50367	1.46%	0.102%
14	9.313	1183	1186	1188	rVB2	56062	49174	1.42%	0.100%
15	9.377	1193	1197	1201	rBV	3816822	3458264	100.00%	7.021%
16	9.448	1207	1209	1213	rVB3	76756	81616	2.36%	0.166%
17	9.636	1238	1241	1243	rBV2	100300	78563	2.27%	0.160%
18	9.772	1261	1264	1272	rVB	430619	408604	11.82%	0.830%
19	9.830	1272	1274	1278	rBV4	38121	43027	1.24%	0.087%
20	9.930	1288	1291	1294	rBV	77109	71580	2.07%	0.145%
21	9.977	1297	1299	1304	rVB	135694	118161	3.42%	0.240%
22	10.072	1311	1315	1319	rVV2	2466981	2124614	61.44%	4.313%
23	10.101	1319	1320	1323	rVB	48280	39451	1.14%	0.080%
24	10.219	1336	1340	1342	rBV5	31967	52282	1.51%	0.106%
25	10.272	1346	1349	1352	rVV4	53665	55127	1.59%	0.112%
26	10.307	1352	1355	1359	rBV3	58944	79108	2.29%	0.161%
27	10.383	1365	1368	1371	rBV4	72849	95202	2.75%	0.193%
28	10.483	1381	1385	1388	rBV	199794	183090	5.29%	0.372%
29	10.619	1406	1408	1411	rVB2	55835	45987	1.33%	0.093%
30	10.701	1418	1422	1425	rBV2	174186	219460	6.35%	0.446%
31	10.866	1446	1450	1454	rBV	1763649	1632840	47.22%	3.315%
32	10.971	1463	1468	1475	rVB2	274910	459783	13.30%	0.933%
33	11.407	1540	1542	1545	rBV	214861	175816	5.08%	0.357%
34	11.436	1545	1547	1550	rVV	173540	160400	4.64%	0.326%

LSC Area Percent Report

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Data File : BF108115.D
Acq On : 13 Aug 2018 14:49
Operator : JU/SJ
Sample : J4272-15 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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	11.571	1566	1570	1572	rBV	2227974	1881089	54.39%	3.819%
36	11.595	1572	1574	1577	rVB	643961	475326	13.74%	0.965%
37	11.648	1580	1583	1587	rVV	179450	155112	4.49%	0.315%
38	11.718	1593	1595	1599	rBV3	57694	70374	2.03%	0.143%
39	11.795	1605	1608	1610	rBV3	74452	76555	2.21%	0.155%
40	11.836	1613	1615	1618	rVB	213710	165632	4.79%	0.336%
41	11.942	1629	1633	1636	rVB	1102684	923630	26.71%	1.875%
42	12.077	1652	1656	1658	rBV	256735	263580	7.62%	0.535%
43	12.101	1658	1660	1664	rVB2	176994	146717	4.24%	0.298%
44	12.148	1666	1668	1672	rVB2	71518	65299	1.89%	0.133%
45	12.189	1672	1675	1677	rBV2	159265	162025	4.69%	0.329%
46	12.248	1682	1685	1688	rBV	187876	156907	4.54%	0.319%
47	12.371	1703	1706	1708	rVB	69233	59670	1.73%	0.121%
48	12.401	1708	1711	1714	rBV4	89308	97014	2.81%	0.197%
49	12.636	1747	1751	1752	rBV	2600568	2416591	69.88%	4.906%
50	12.654	1752	1754	1762	rVB	2798037	2535909	73.33%	5.148%
51	12.713	1762	1764	1765	rBV	67307	56518	1.63%	0.115%
52	12.736	1765	1768	1773	rVV	762905	658266	19.03%	1.336%
53	12.795	1774	1778	1781	rVV	1263022	1118352	32.34%	2.271%
54	12.824	1781	1783	1786	rVB2	121593	119228	3.45%	0.242%
55	13.024	1811	1817	1822	rVB	1128395	1311125	37.91%	2.662%
56	13.071	1823	1825	1828	rVV2	81628	69502	2.01%	0.141%
57	13.160	1836	1840	1843	rVB	3127946	2651639	76.68%	5.383%
58	13.583	1909	1912	1915	rBV3	227664	227578	6.58%	0.462%
59	14.071	1992	1995	2004	rVB2	247417	387725	11.21%	0.787%
60	14.230	2017	2022	2025	rBV2	2242264	2531327	73.20%	5.139%
61	14.254	2025	2026	2033	rVB	475079	430061	12.44%	0.873%
62	15.330	2207	2209	2213	rBV	255997	363681	10.52%	0.738%
63	15.812	2286	2291	2295	rBV2	1164153	1648410	47.67%	3.347%

Sum of corrected areas: 49255327

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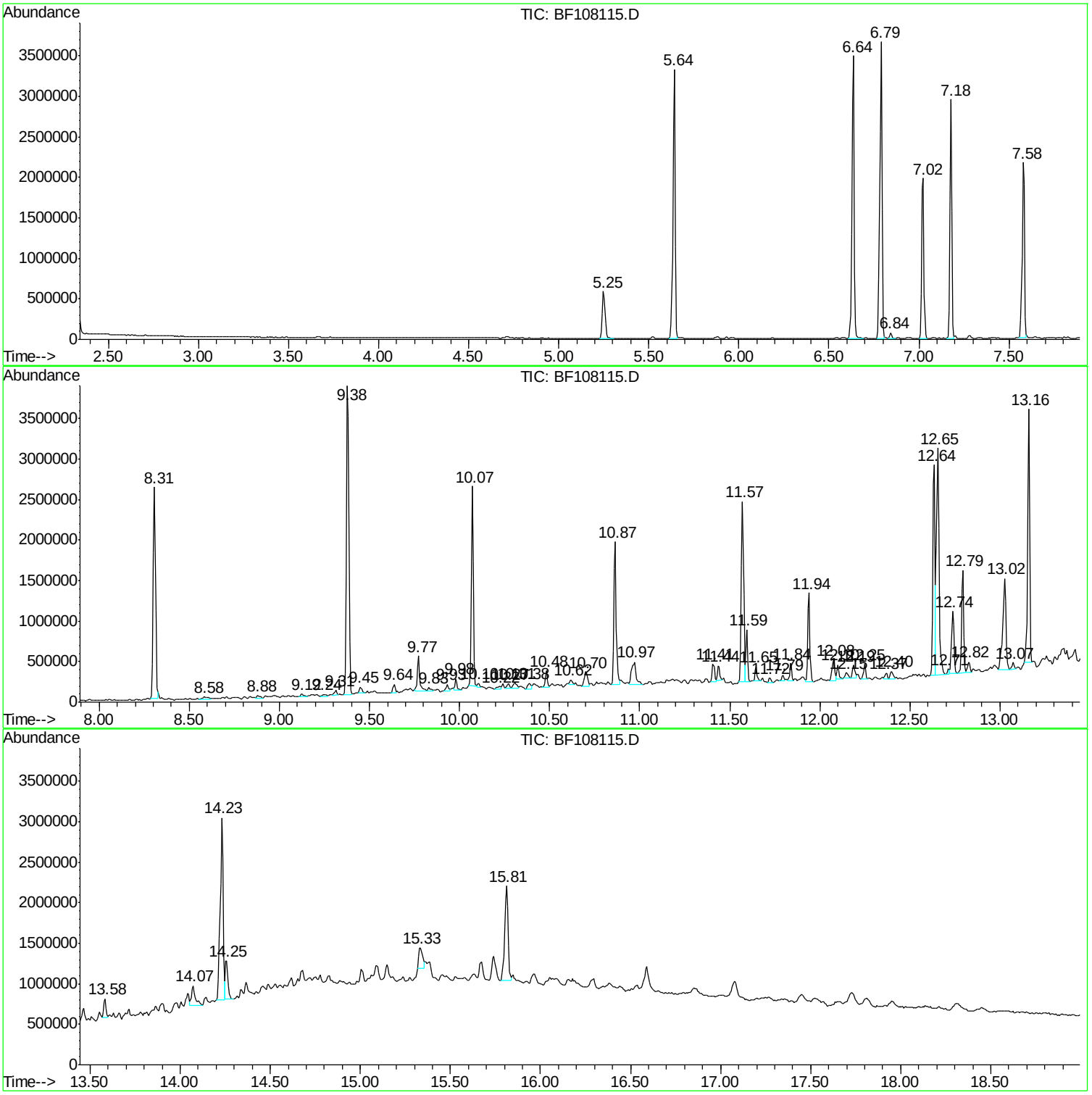
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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

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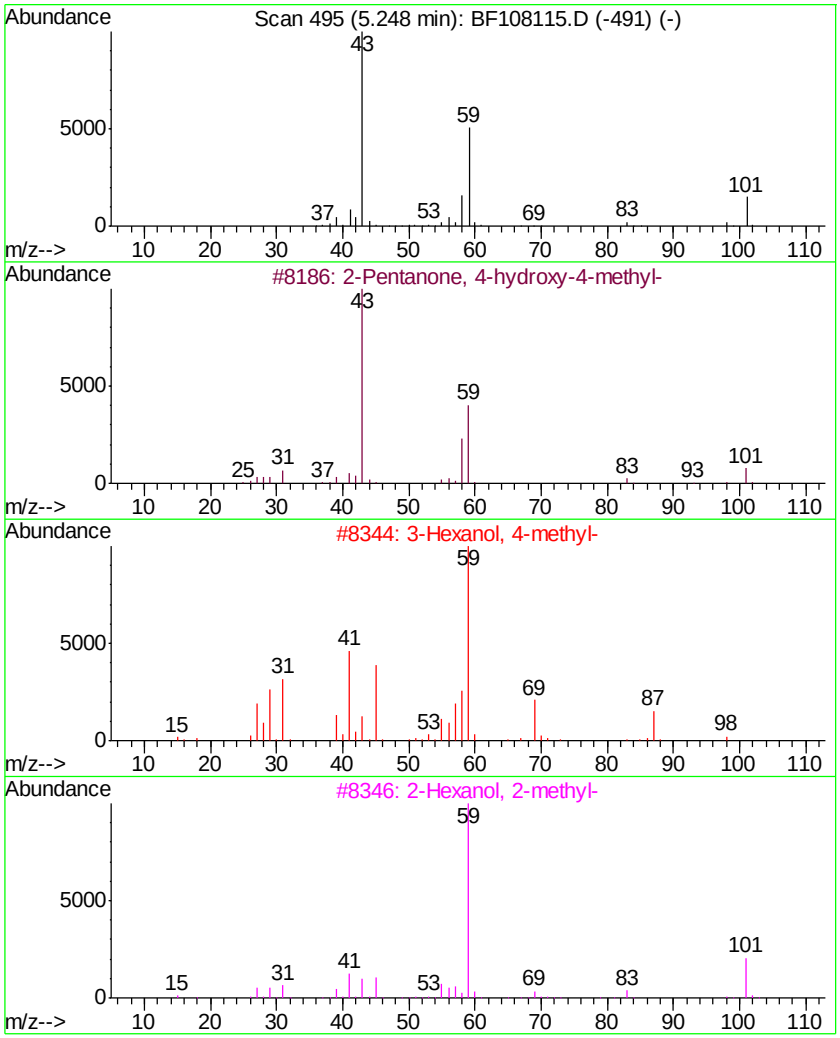
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

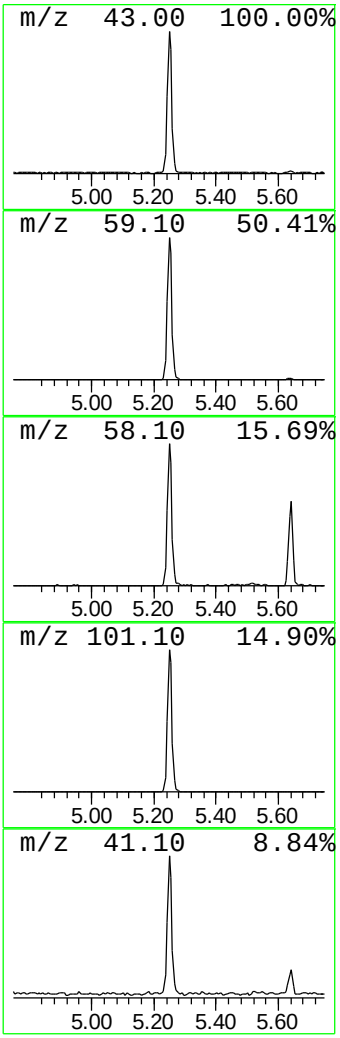
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	6.86 ng	606739	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	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
Data File : BF108115.D
Acq On : 13 Aug 2018 14:49
Operator : JU/SJ
Sample : J4272-15 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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

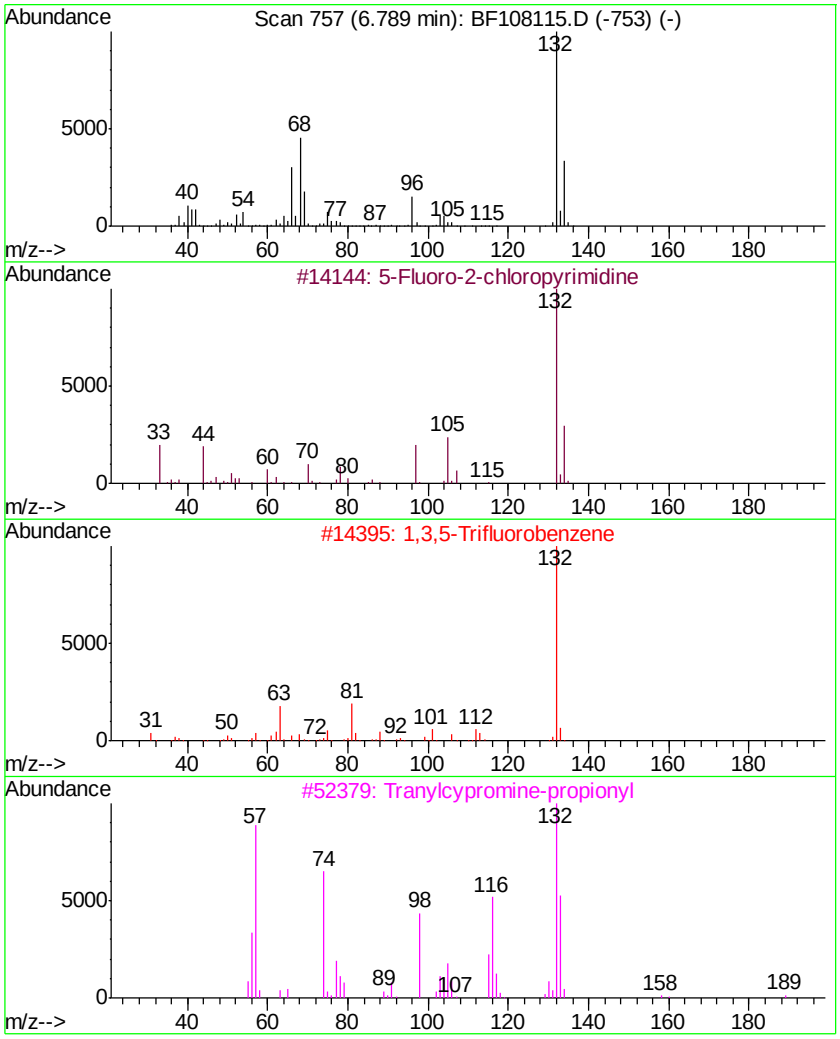
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

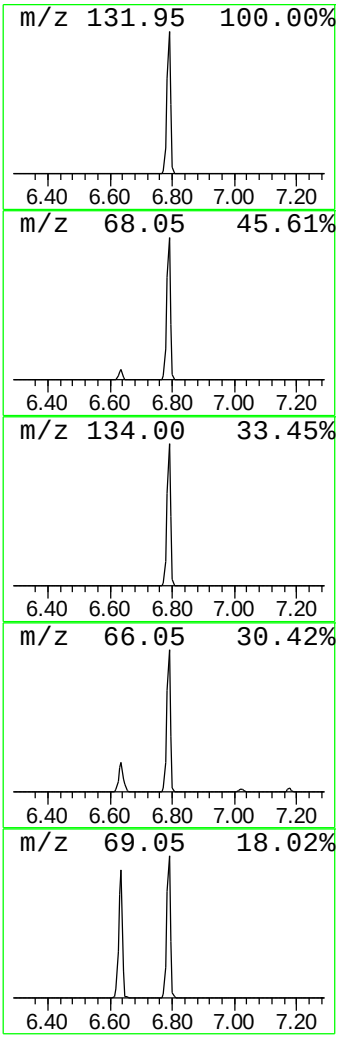
****

Peak Number 2 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	35.02 ng	3095390	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	12
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	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 :
ALS Vial : 8 Sample Multiplier: 1

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

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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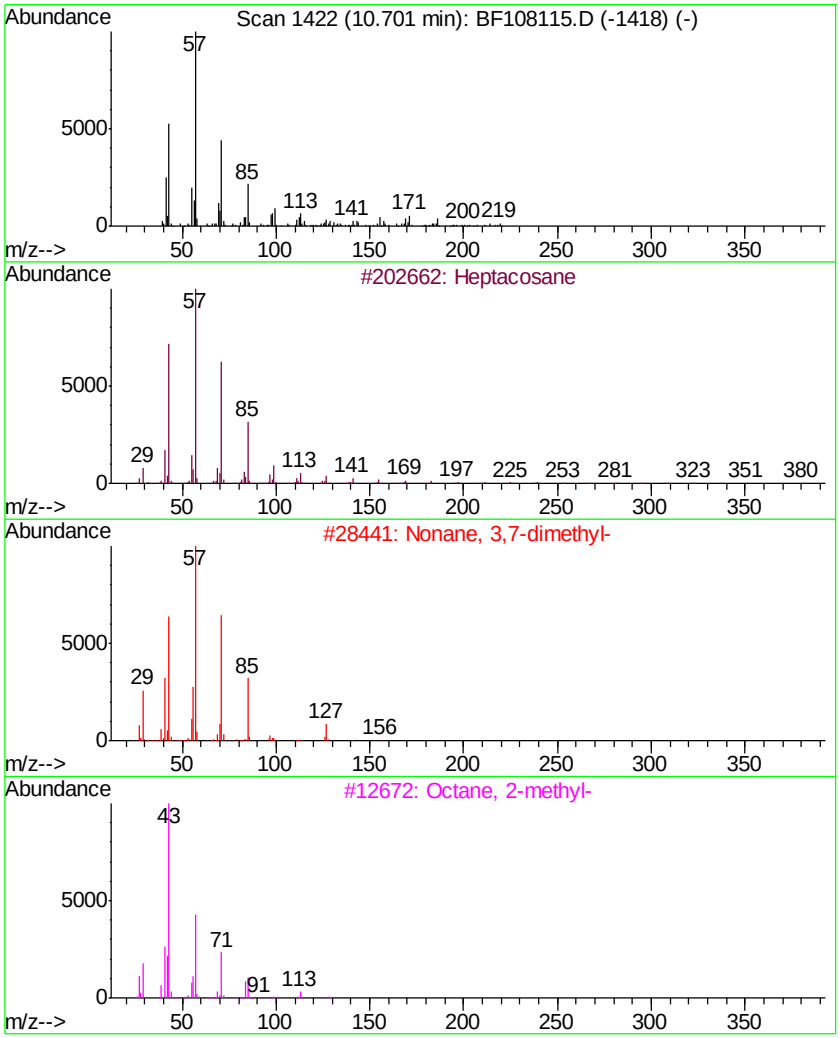
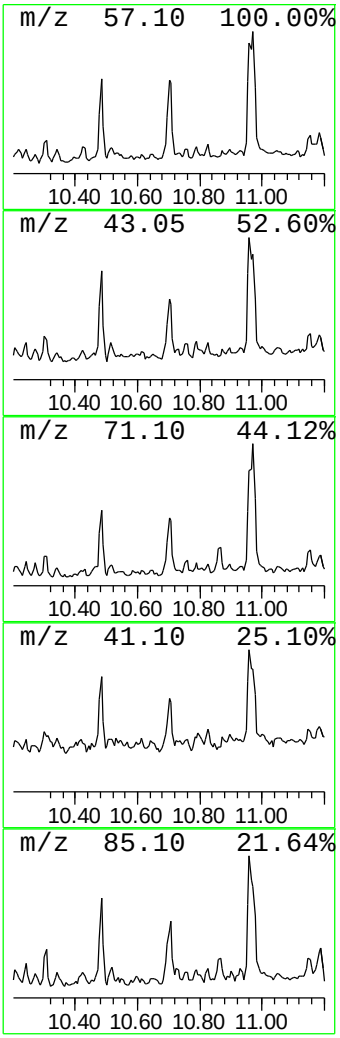
Peak Number 4 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.07 ng	219460	Acenaphthene-d10	10.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	68
2	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
3	Octane, 2-methyl-	128	C9H20	003221-61-2	64
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
5	Tridecane	184	C13H28	000629-50-5	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
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Misc :
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Instrument : BNA_F
ClientSampleId : JC-03-080918-H

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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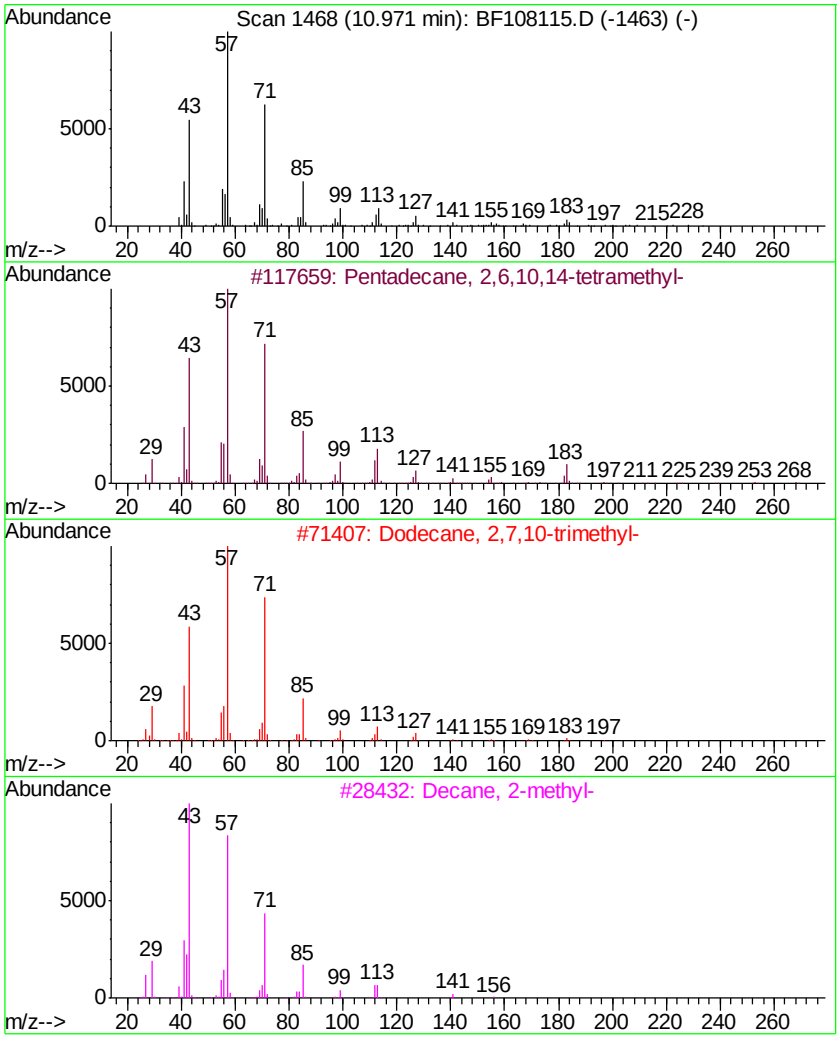
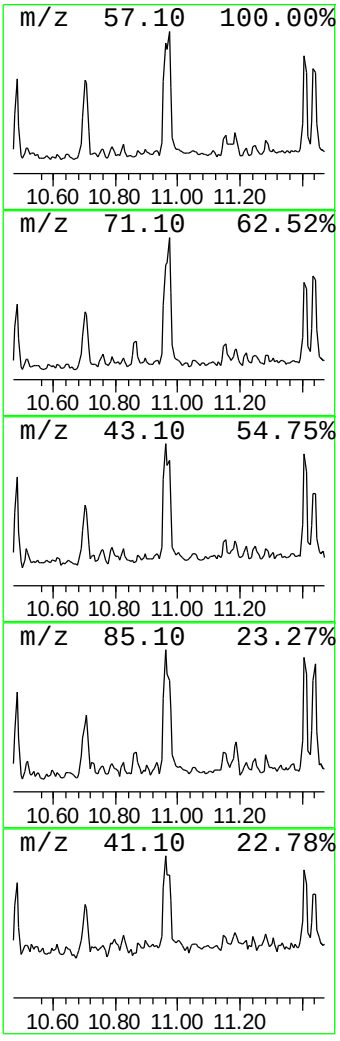
****

Peak Number 5 Pentadecane, 2,6,10,14-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	4.89 ng	459783	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
3	Decane, 2-methyl-	156	C11H24	006975-98-0	74
4	Tridecane	184	C13H28	000629-50-5	72
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	72





Library Search Compound Report

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

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

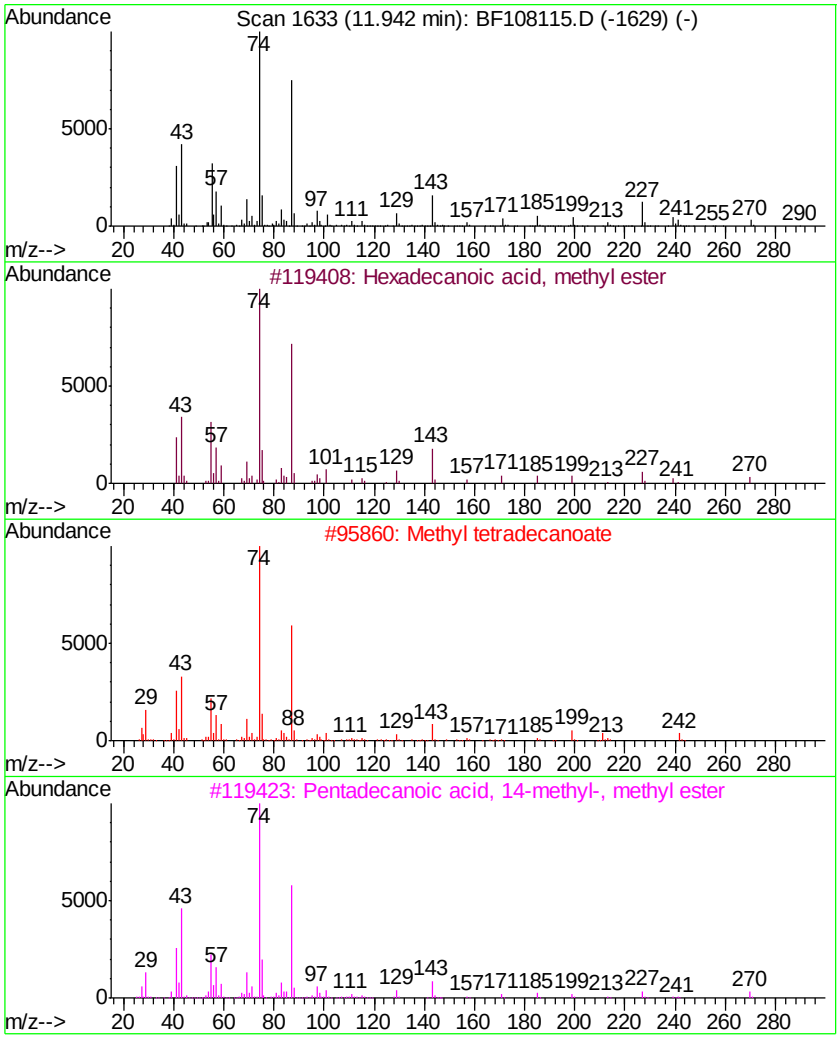
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

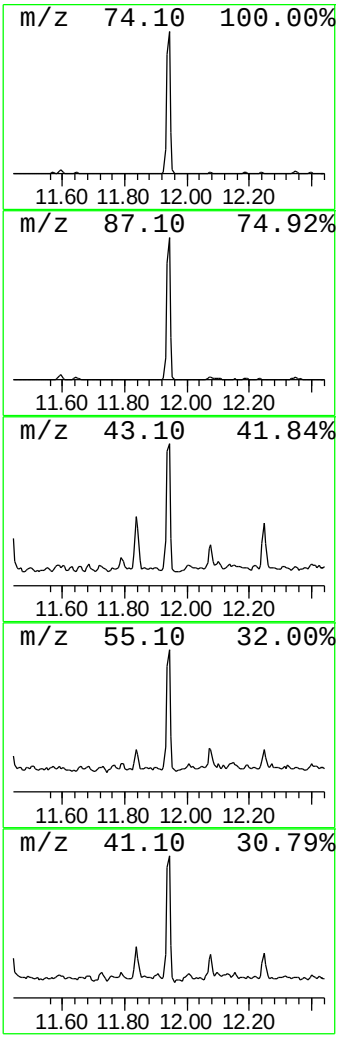
****

Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	9.82 ng	923630	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87





Library Search Compound Report

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Misc :
ALS Vial : 8 Sample Multiplier: 1

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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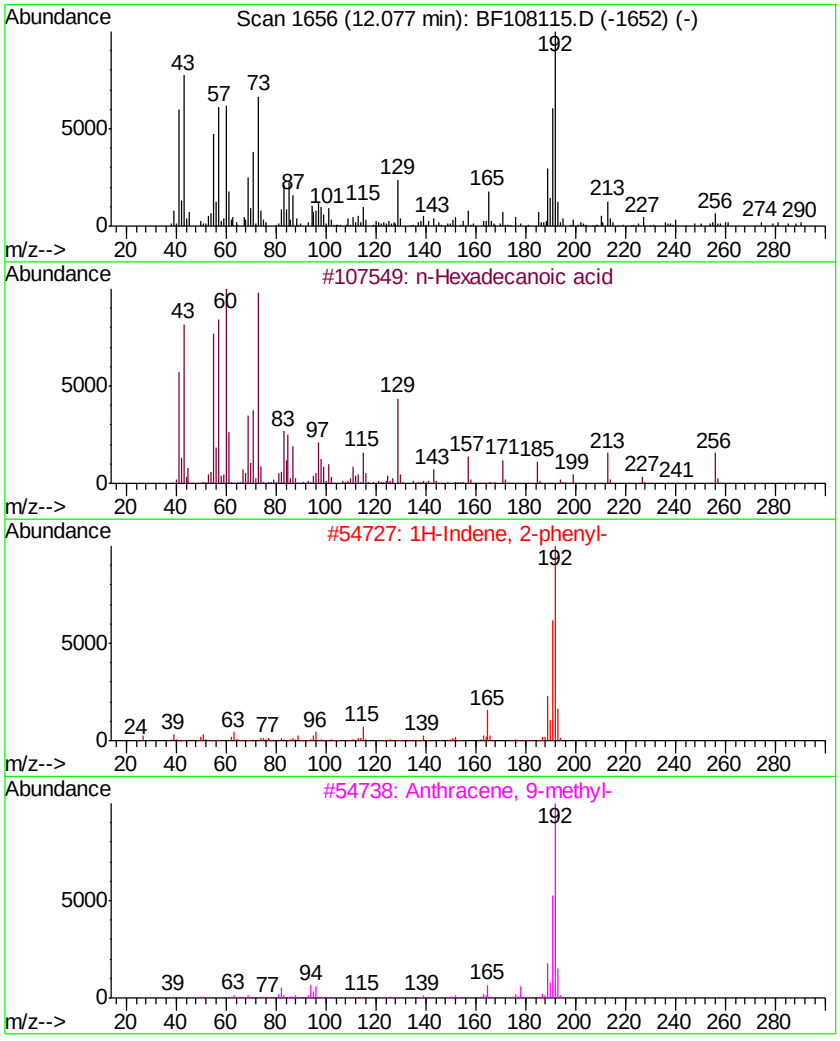
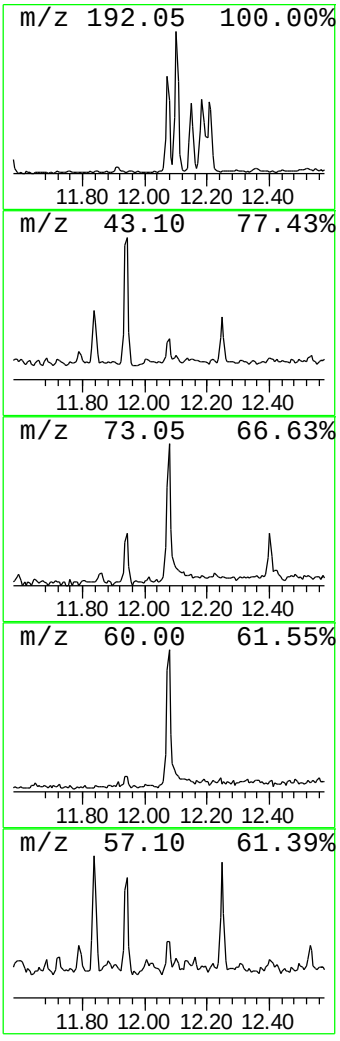
Peak Number 7 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	2.80 ng	263580	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	81
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	58
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	55
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	52





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
Data File : BF108115.D
Acq On : 13 Aug 2018 14:49
Operator : JU/SJ
Sample : J4272-15 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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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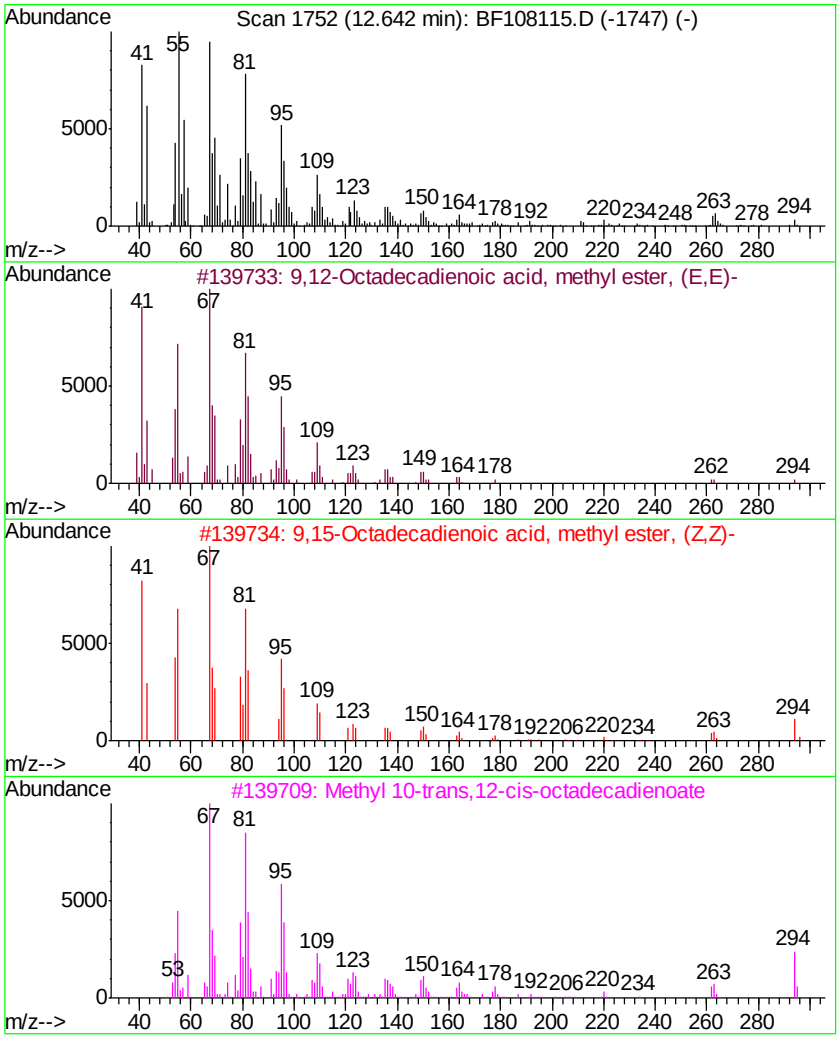
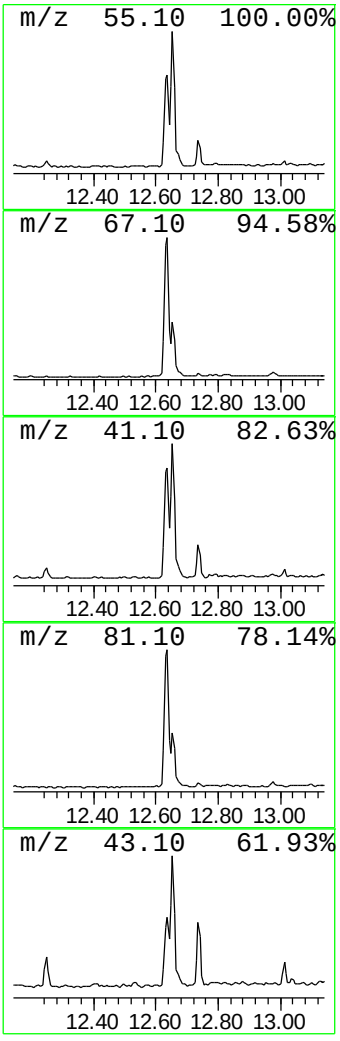
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	25.69 ng	2416590	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	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	98
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	97





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
Data File : BF108115.D
Acq On : 13 Aug 2018 14:49
Operator : JU/SJ
Sample : J4272-15 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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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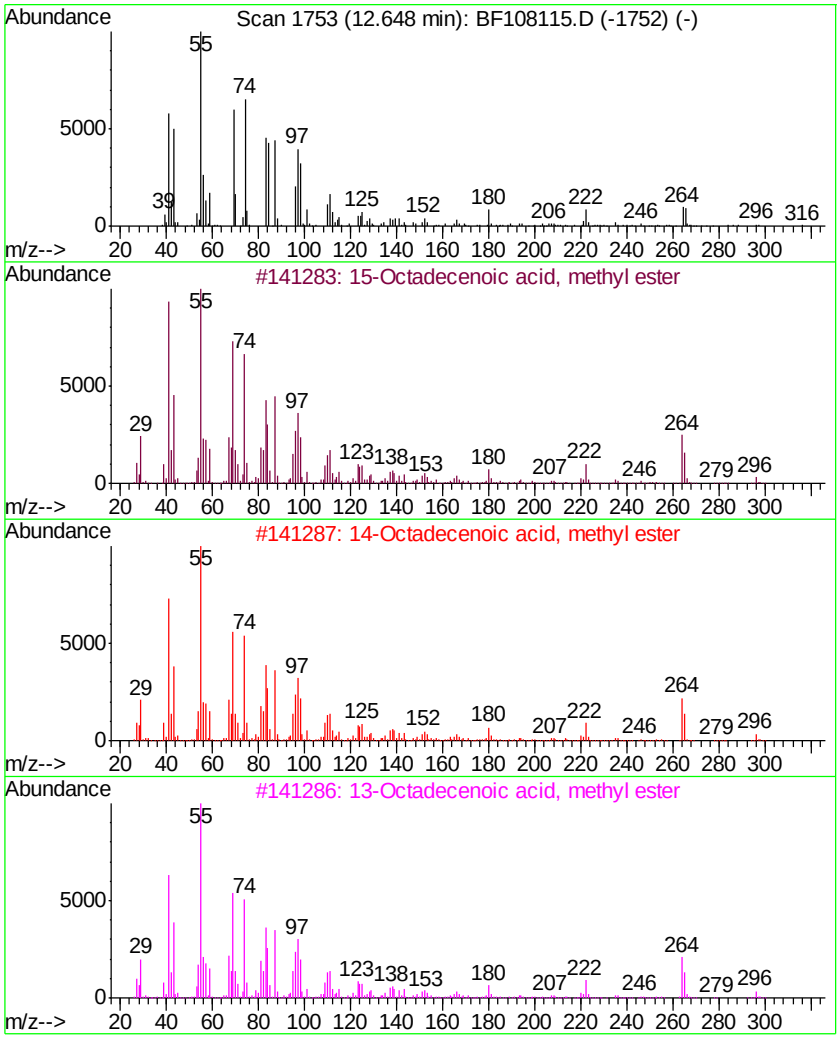
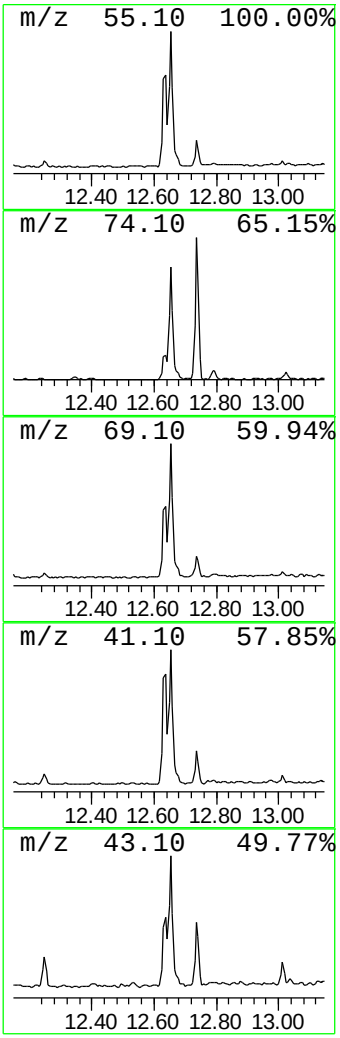
Peak Number 9 15-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	26.96 ng	2535910	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	96
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	95
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	95
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94





Library Search Compound Report

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

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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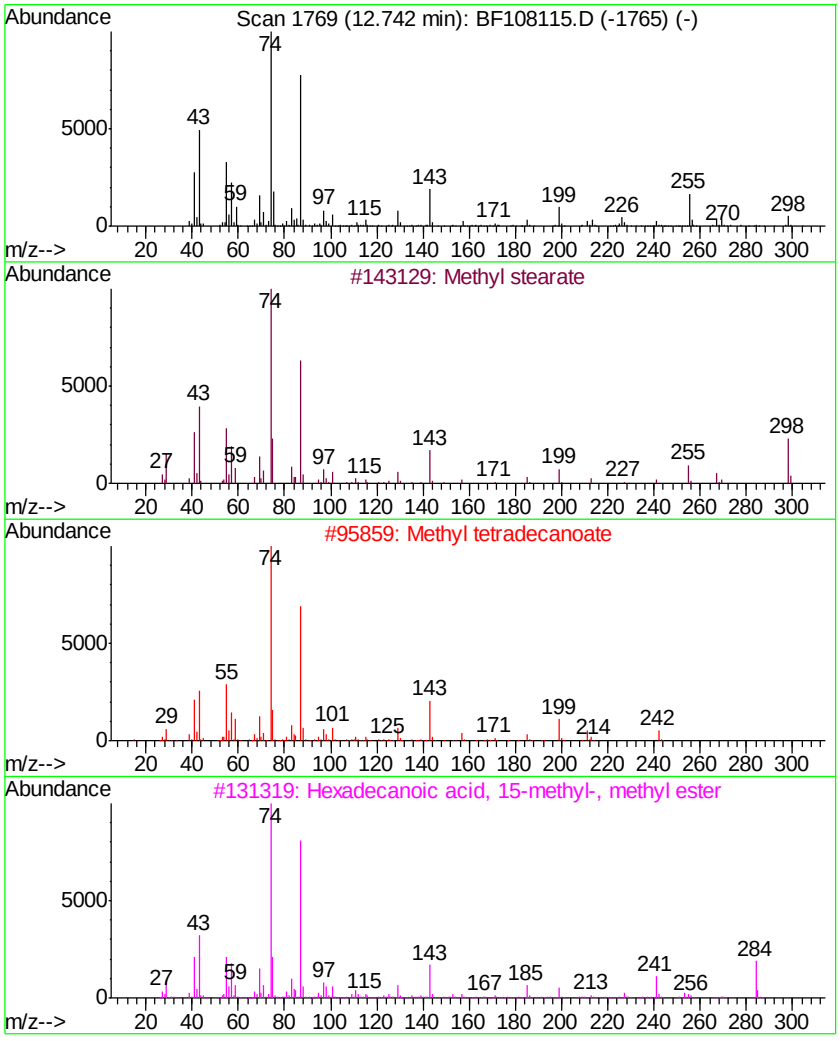
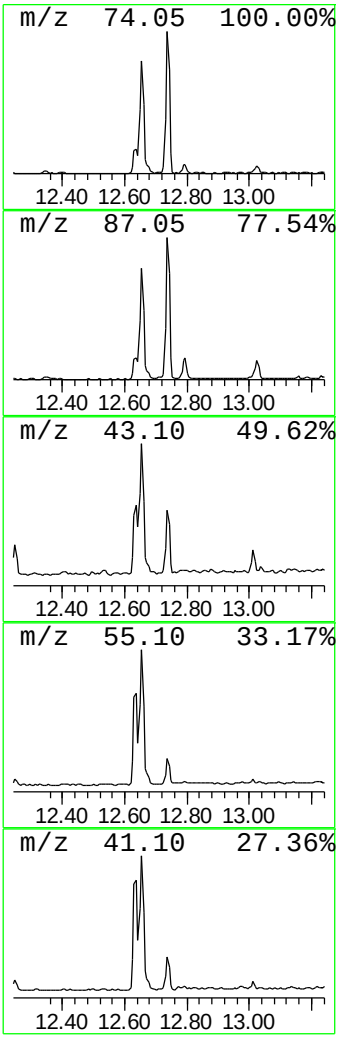
Peak Number 10 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	7.00 ng	658266	Phenanthrene-d10	11.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





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Sample : J4272-15 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Integration Parameters: LSCINT.P

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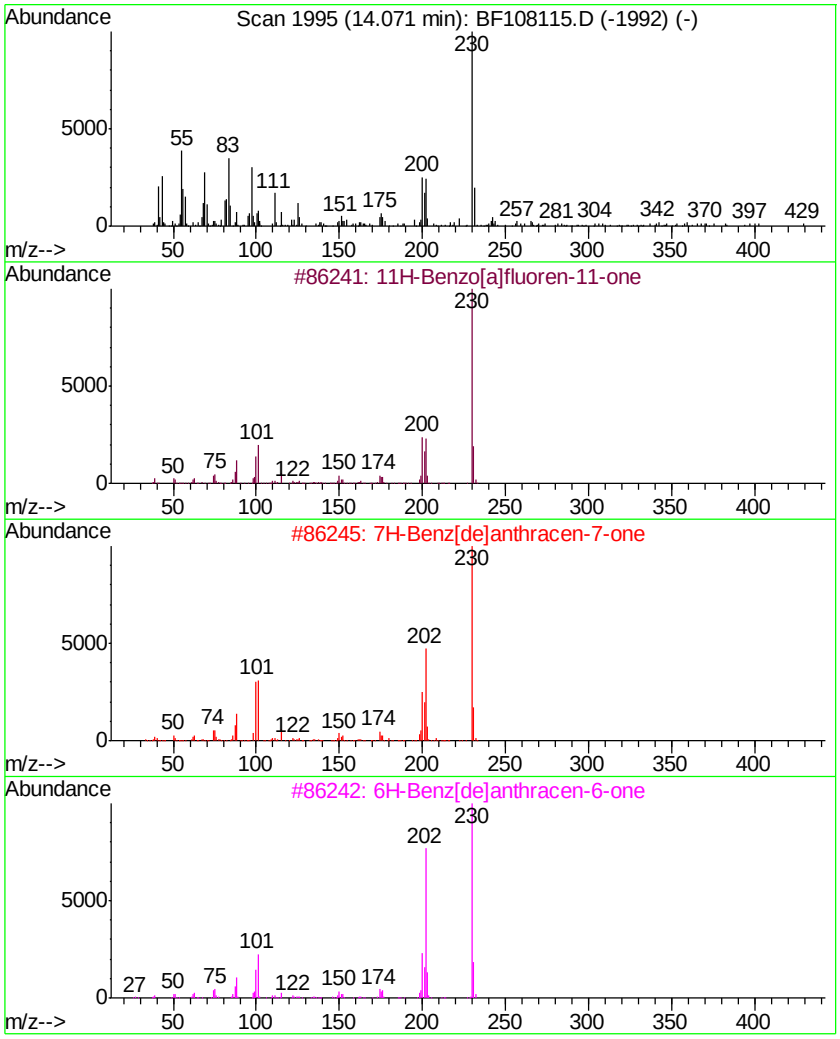
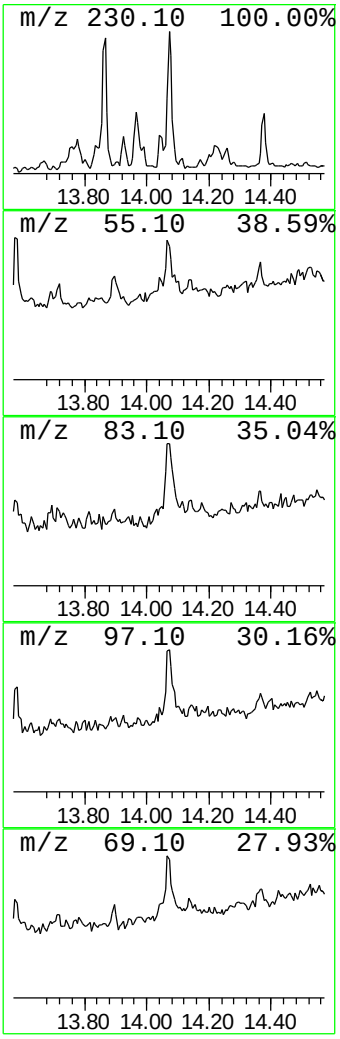
Peak Number 11 11H-Benzo[a]fluoren-11-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	3.06 ng	387725	Chrysene-d12	14.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	95
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	62
3	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	52
4	o-Terphenyl	230	C18H14	000084-15-1	47
5	p-Terphenyl	230	C18H14	000092-94-4	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081318\
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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	6.9	ng	606739	1	7.02	1767700	20.0
unknown6.79	6.79	35.0	ng	3095390	1	7.02	1767700	20.0
Heptacosane	10.70	2.1	ng	219460	3	10.07	2124610	20.0
Pentadecane, 2,6,...	10.97	4.9	ng	459783	4	11.57	1881090	20.0
Hexadecanoic acid...	11.94	9.8	ng	923630	4	11.57	1881090	20.0
n-Hexadecanoic acid	12.08	2.8	ng	263580	4	11.57	1881090	20.0
9,12-Octadecadien...	12.64	25.7	ng	2416590	4	11.57	1881090	20.0
15-Octadecenoic a...	12.65	27.0	ng	2535910	4	11.57	1881090	20.0
Methyl stearate	12.74	7.0	ng	658266	4	11.57	1881090	20.0
11H-Benzo[a]fluor...	14.07	3.1	ng	387725	5	14.23	2531330	20.0