LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109350.D
Acq On : 26 Sep 2018 21:14
Operator : JU/SJ
Sample : J4773-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092518-E

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-BF092218.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	4.898	474	478	488	rVB	51632	64503	3.74%	0.351%
2	5.316	545	549	553	rBV	1725438	1641584	95.30%	8.944%
3	6.345	719	724	727	rBV	1840229	1709112	99.22%	9.312%
4	6.475	742	746	749	rBV	2005498	1720056	99.85%	9.372%
5	6.704	782	785	789	rBV	657973	572510	33.24%	3.119%
6	6.863	808	812	815	rBV	1669489	1321975	76.74%	7.203%
7	7.269	876	881	884	rBV	1095847	1047773	60.83%	5.709%
8	7.986	999	1003	1009	rBV	828382	692471	40.20%	3.773%
9	9.063	1182	1186	1189	rBV	2205448	1722576	100.00%	9.386%
10	9.457	1249	1253	1256	rBV	522007	404779	23.50%	2.206%
11	9.739	1297	1301	1304	rBV	750812	660944	38.37%	3.601%
12	10.522	1430	1434	1441	rBV	1053426	899723	52.23%	4.902%
13	10.651	1454	1456	1464	rBV2	17435	21675	1.26%	0.118%
14	11.216	1548	1552	1554	rBV	731585	598908	34.77%	3.263%
15	11.239	1554	1556	1559	rVV	58822	47247	2.74%	0.257%
16	11.286	1559	1564	1569	rVB	24920	24732	1.44%	0.135%
17	11.621	1618	1621	1626	rVB	187327	143519	8.33%	0.782%
18	11.751	1639	1643	1647	rBV2	77246	78047	4.53%	0.425%
19	11.827	1653	1656	1658	rBV	31755	33342	1.94%	0.182%
20	12.263	1726	1730	1733	rBV	22902	25163	1.46%	0.137%
21	12.304	1733	1737	1738	rBV	361727	299429	17.38%	1.631%
22	12.321	1738	1740	1743	rVB	349026	273688	15.89%	1.491%
23	12.421	1752	1757	1761	rBV2	183149	203675	11.82%	1.110%
24	12.645	1790	1795	1799	rBV	194374	185788	10.79%	1.012%
25	12.798	1817	1821	1824	rBV	1664834	1512368	87.80%	8.240%
26	12.868	1828	1833	1835	rBV4	16888	25112	1.46%	0.137%
27	12.974	1844	1851	1855	rBV	35594	56234	3.26%	0.306%
28	13.039	1860	1862	1866	rVB2	28264	27638	1.60%	0.151%
29	13.080	1866	1869	1871	rBV2	31910	29177	1.69%	0.159%
30	13.204	1887	1890	1893	rBV	22694	21030	1.22%	0.115%
31	13.480	1935	1937	1941	rVB4	19648	24100	1.40%	0.131%
32	13.545	1945	1948	1952	rBV2	23080	29819	1.73%	0.162%
33	13.586	1952	1955	1958	rBV2	21040	24004	1.39%	0.131%
34	13.710	1970	1976	1983	rBV3	74219	128278	7.45%	0.699%

LSC Area Percent Report

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Sample : J4773-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092518-E

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.839	1993	1998	2001	rBV	829617	852430	49.49%	4.645%
36	13.863	2001	2002	2005	rVB	89401	65698	3.81%	0.358%
37	14.227	2062	2064	2067	rVB	30360	21540	1.25%	0.117%
38	14.321	2078	2080	2083	rBV2	27856	24057	1.40%	0.131%
39	14.621	2129	2131	2136	rBV3	30324	33890	1.97%	0.185%
40	14.686	2139	2142	2146	rVB	248933	248341	14.42%	1.353%
41	14.845	2166	2169	2177	rVB	83525	149950	8.70%	0.817%
42	15.121	2214	2216	2223	rVB	61559	82552	4.79%	0.450%
43	15.186	2223	2227	2232	rBV	61231	87305	5.07%	0.476%
44	15.239	2232	2236	2240	rBV	458294	516286	29.97%	2.813%

Sum of corrected areas: 18353028

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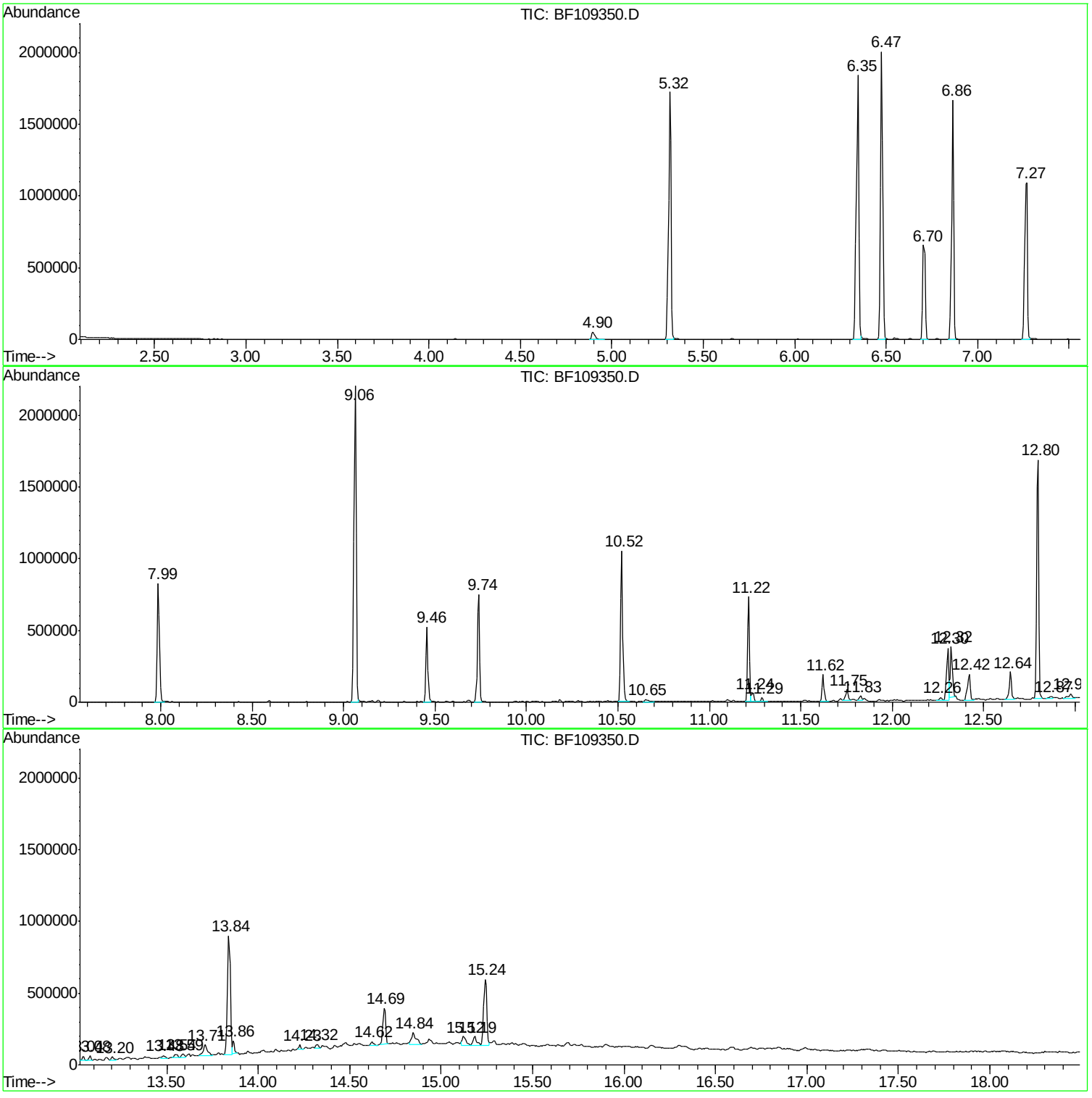
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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Data File : BF109350.D
Acq On : 26 Sep 2018 21:14
Operator : JU/SJ
Sample : J4773-19
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

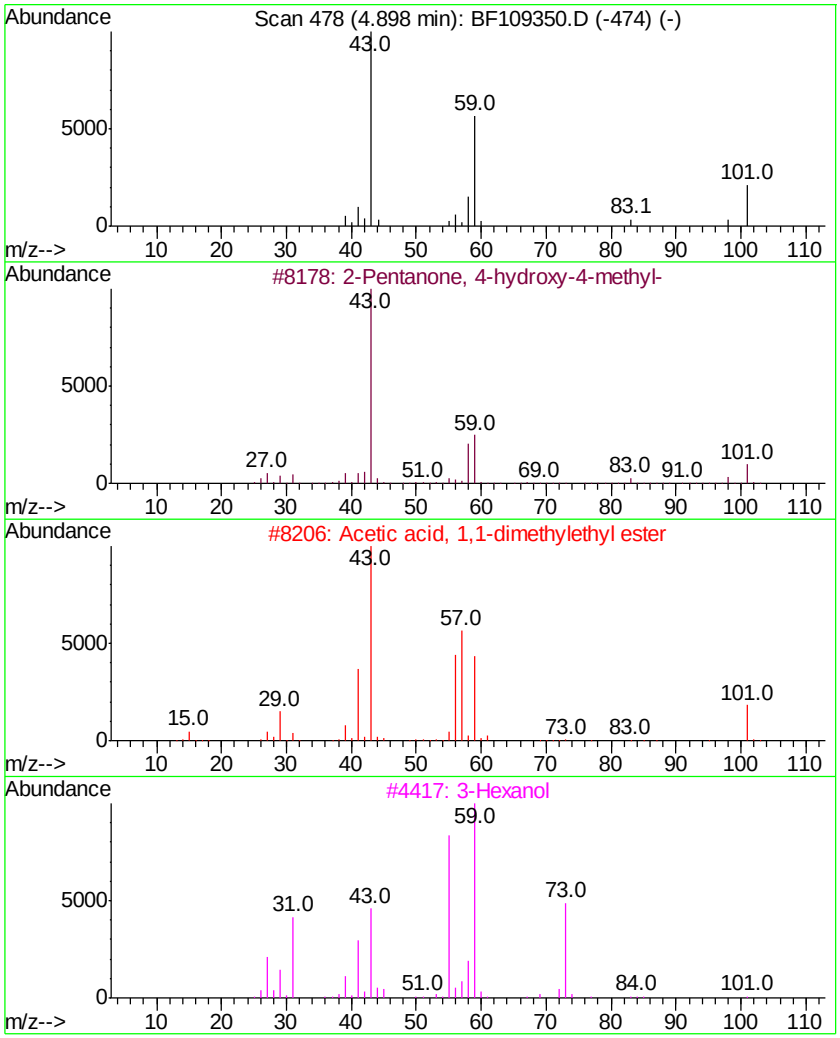
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

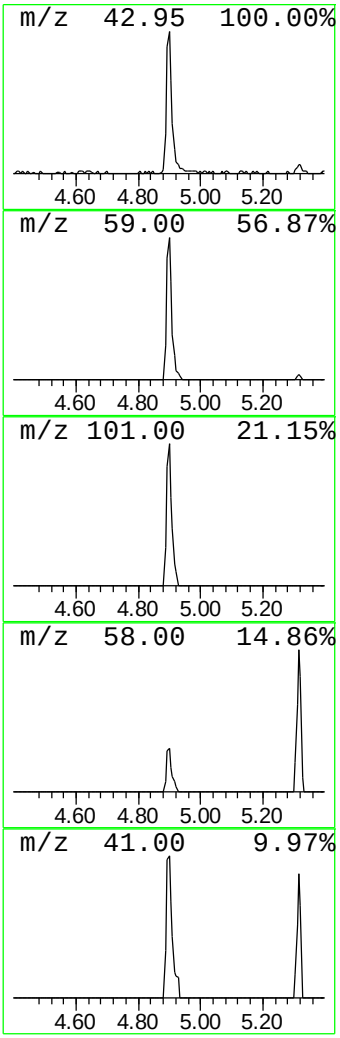
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.25 ng	64503	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF109350.D
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Operator : JU/SJ
Sample : J4773-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
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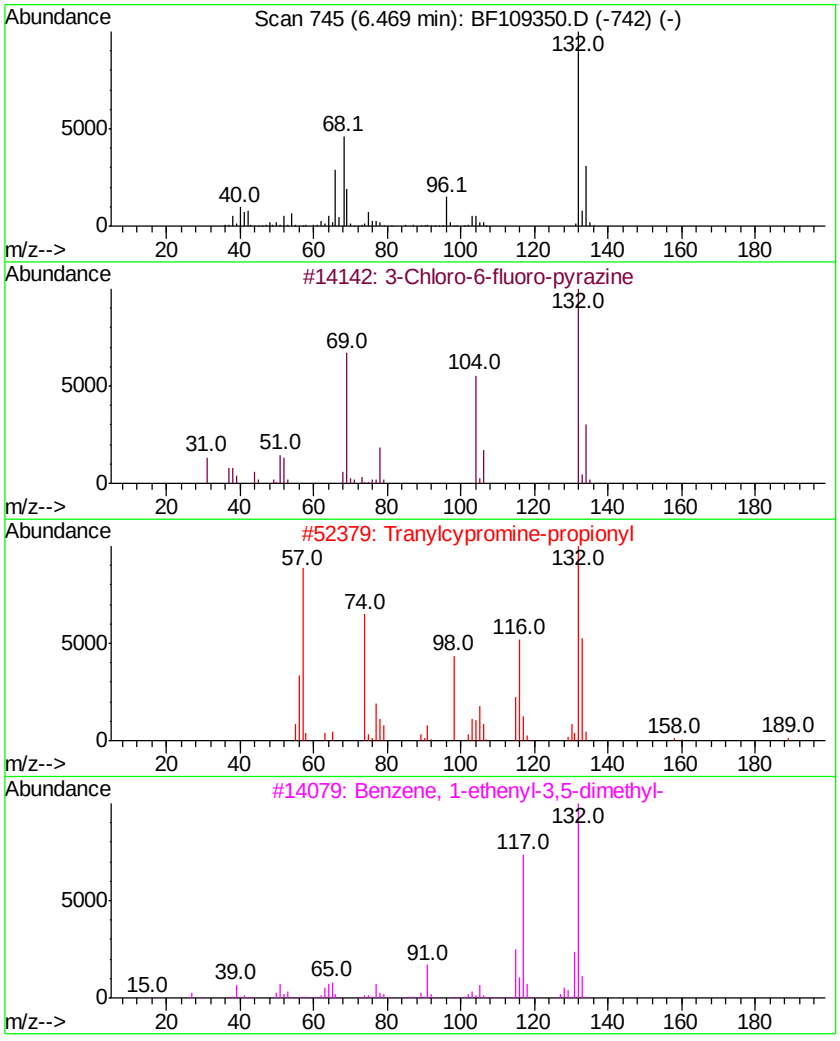
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

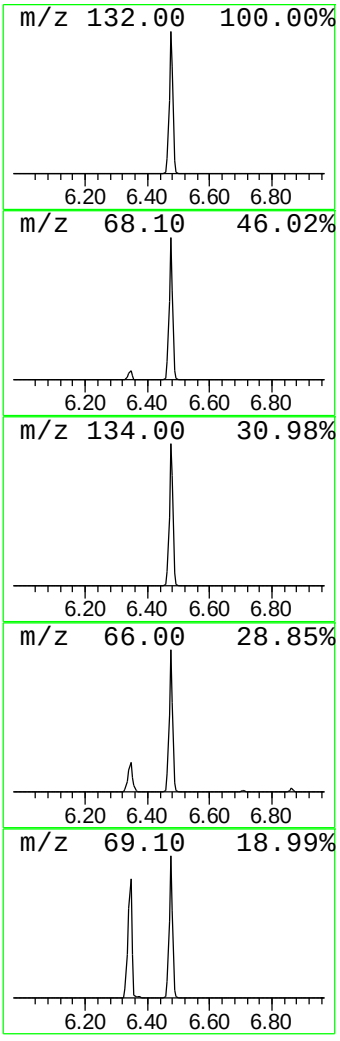
****

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	60.09 ng	1720060	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Data File : BF109350.D
Acq On : 26 Sep 2018 21:14
Operator : JU/SJ
Sample : J4773-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

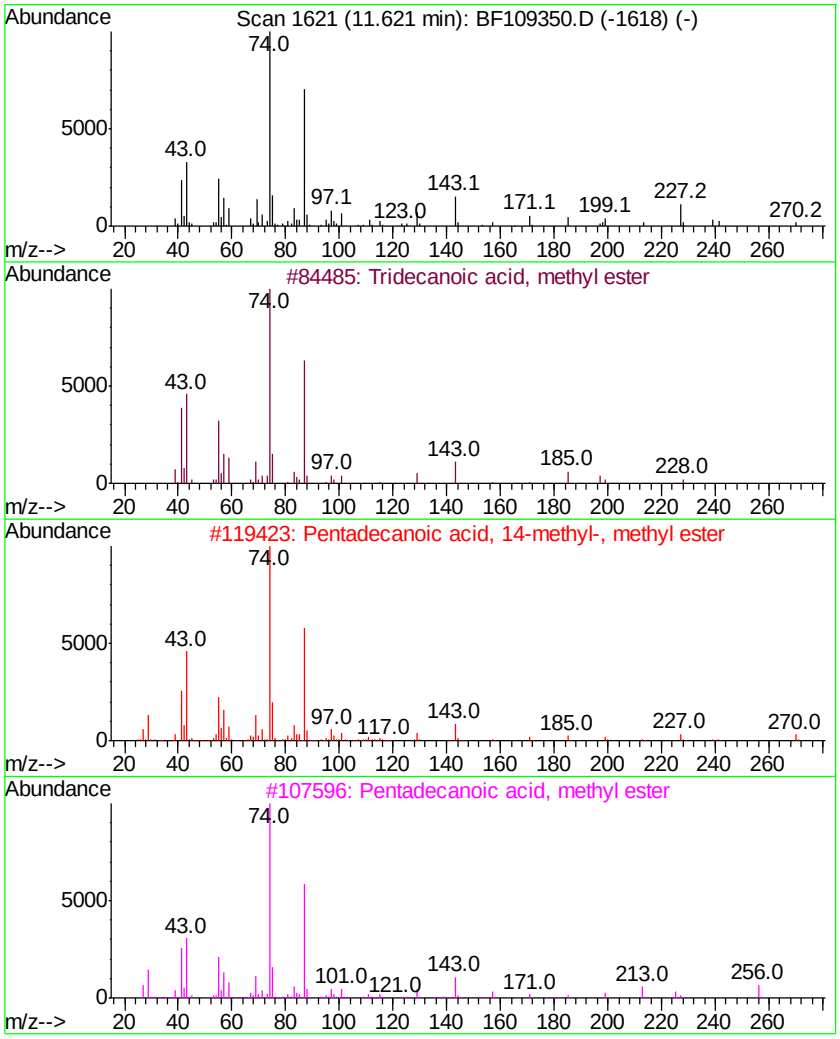
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

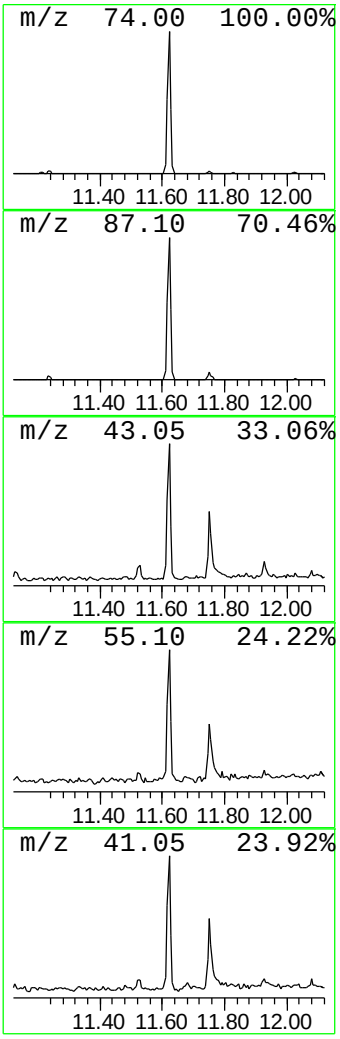
****

Peak Number 4 Tridecanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	4.79 ng	143519	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83





Library Search Compound Report

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Sample : J4773-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
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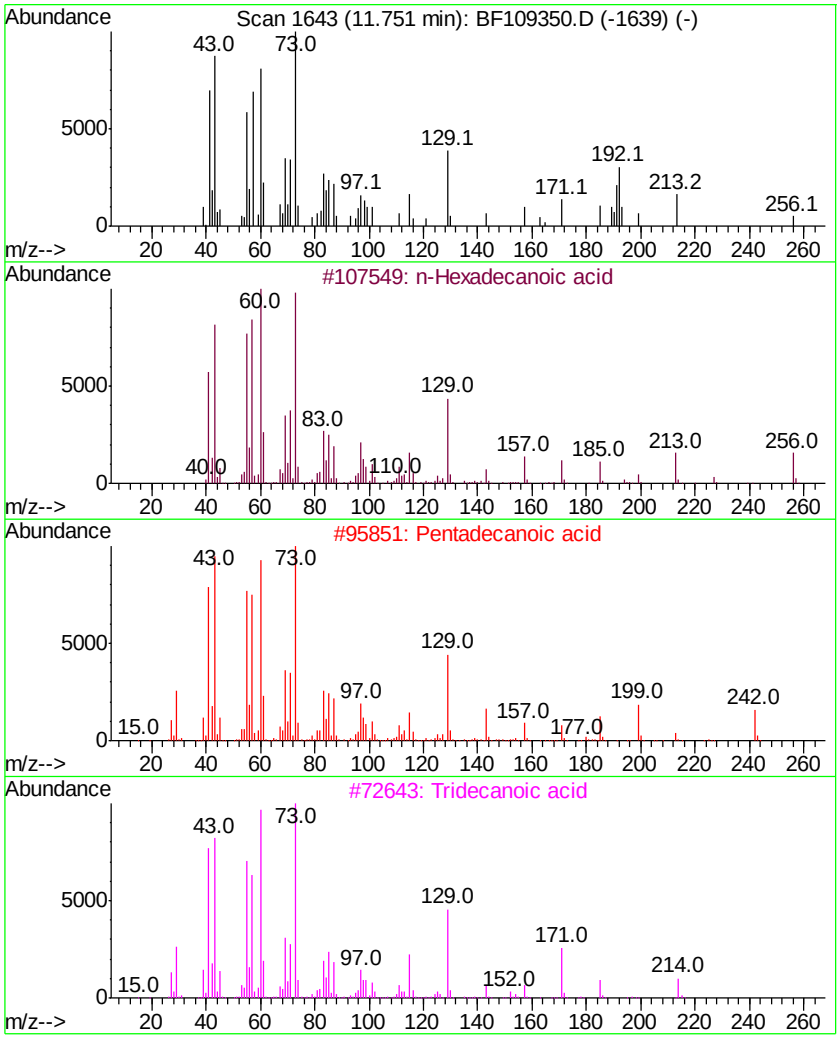
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

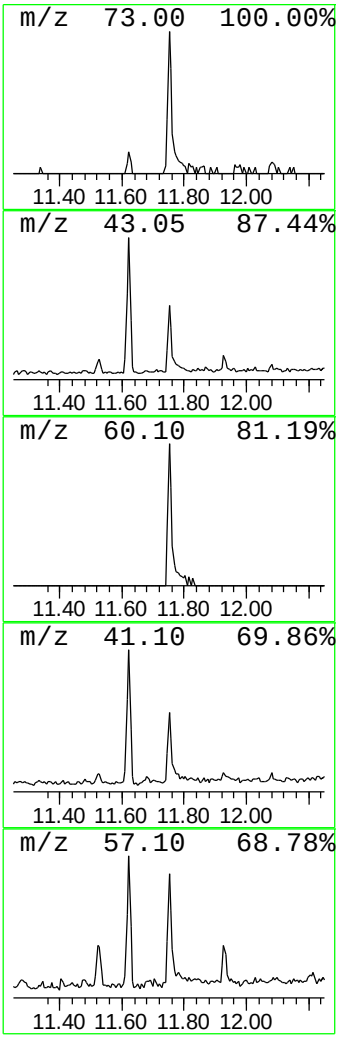
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.61 ng	78047	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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Instrument : BNA_F
ClientSampleId : CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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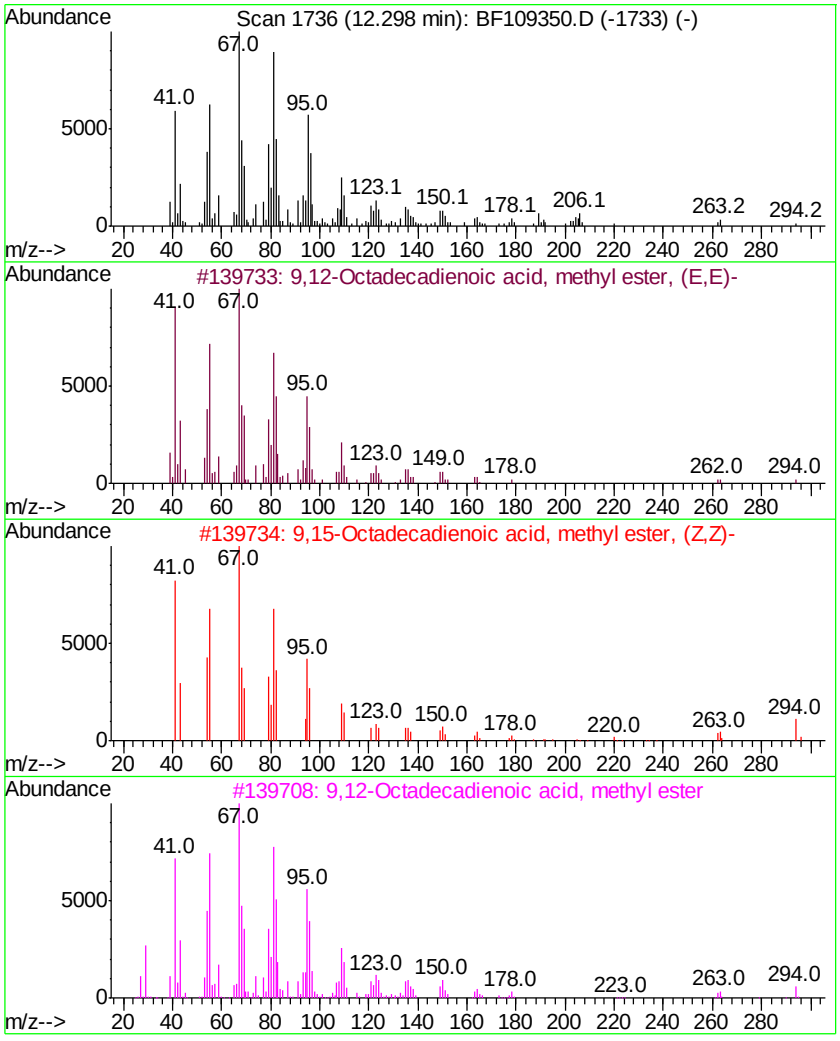
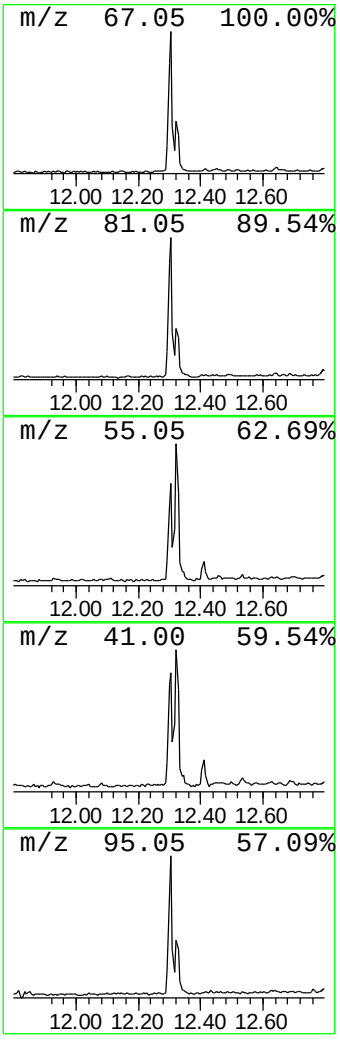
****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	10.00 ng	299429	Phenanthrene-d10	11.22

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	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	97





Library Search Compound Report

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ClientSampleId : CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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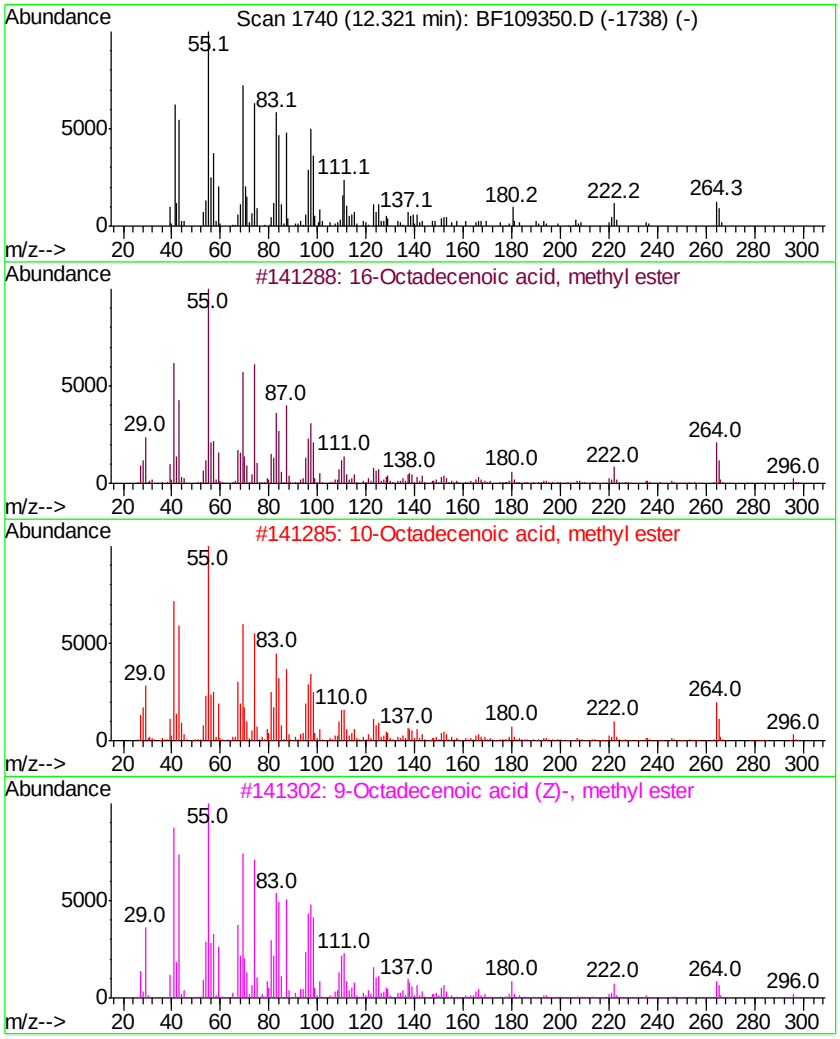
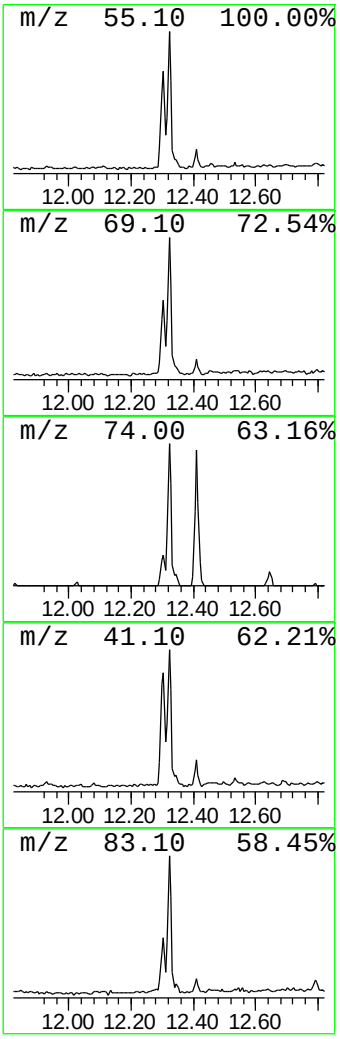
****

Peak Number 7 16-Octadecenoic acid, methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	9.14 ng	273688	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	83
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	76
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	74
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	68





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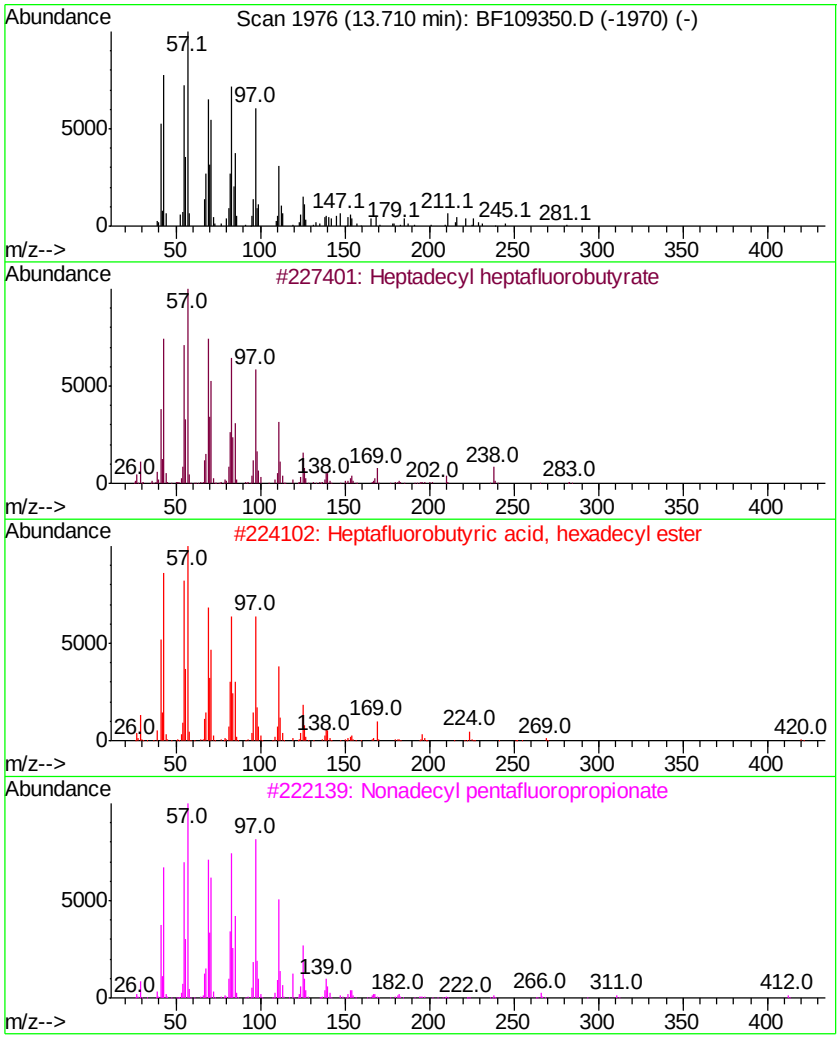
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

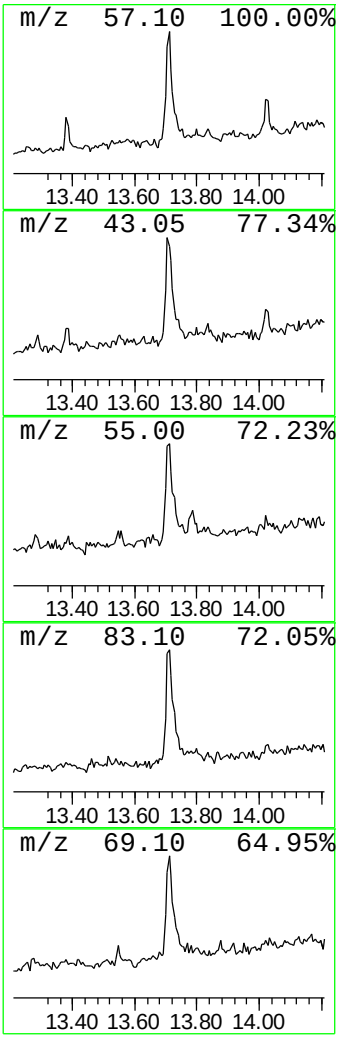
****

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	3.01 ng	128278	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	90





Library Search Compound Report

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Data File : BF109350.D
Acq On : 26 Sep 2018 21:14
Operator : JU/SJ
Sample : J4773-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

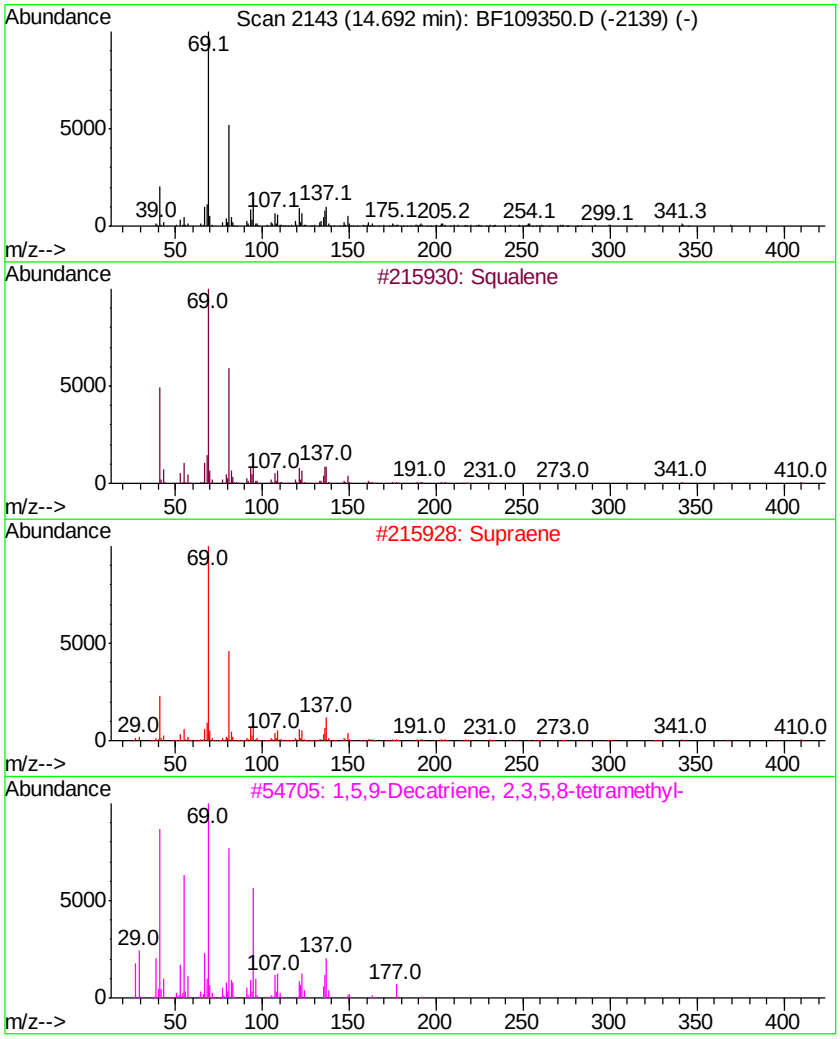
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

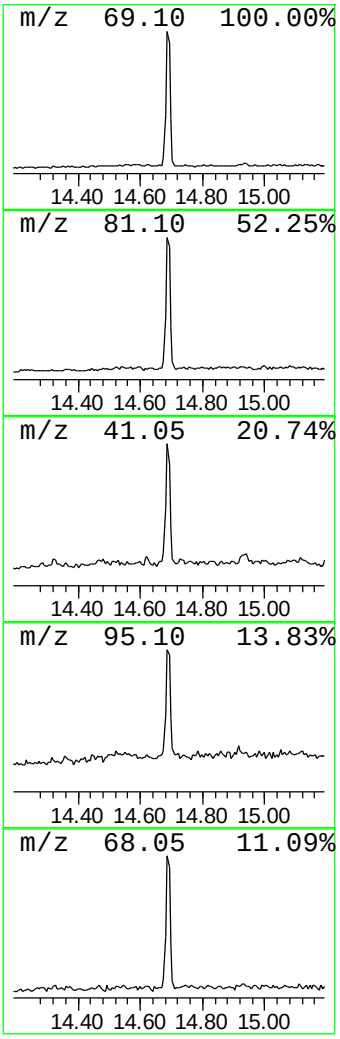
****

Peak Number 9 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	9.62 ng	248341	Perylene-d12	15.24

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	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
4	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092618\
Data File : BF109350.D
Acq On : 26 Sep 2018 21:14
Operator : JU/SJ
Sample : J4773-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092518-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.90	2.3	ng	64503	1	6.70	572510	20.0
unknown6.47	6.47	60.1	ng	1720060	1	6.70	572510	20.0
Tridecanoic acid,...	11.62	4.8	ng	143519	4	11.22	598908	20.0
n-Hexadecanoic acid	11.75	2.6	ng	78047	4	11.22	598908	20.0
9,12-Octadecadien...	12.30	10.0	ng	299429	4	11.22	598908	20.0
16-Octadecenoic a...	12.32	9.1	ng	273688	4	11.22	598908	20.0
Heptadecyl heptaf...	13.71	3.0	ng	128278	5	13.84	852430	20.0
Squalene	14.69	9.6	ng	248341	6	15.24	516286	20.0