LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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	5.310	544	548	558	rBV	225017	204011	19.83%	2.037%
2	6.339	719	723	730	rBV	242240	225983	21.96%	2.256%
3	6.475	742	746	749	rBV	280843	228919	22.25%	2.286%
4	6.710	782	786	789	rBV	861021	712436	69.24%	7.113%
5	6.863	809	812	816	rBV	236126	184037	17.89%	1.837%
6	7.263	877	880	889	rVB	166929	132517	12.88%	1.323%
7	7.992	1000	1004	1007	rBV	1150974	938511	91.21%	9.370%
8	9.063	1183	1186	1192	rBV	360095	277686	26.99%	2.772%
9	9.457	1250	1253	1259	rBV	73672	61441	5.97%	0.613%
10	9.686	1290	1292	1295	rBV	16187	12255	1.19%	0.122%
11	9.739	1297	1301	1305	rBV2	1255924	1028912	100.00%	10.273%
12	9.769	1305	1306	1311	rVB	28196	18764	1.82%	0.187%
13	10.180	1374	1376	1379	rVB	22098	19701	1.91%	0.197%
14	10.286	1391	1394	1400	rVB	20912	23617	2.30%	0.236%
15	10.404	1410	1414	1419	rBV	11572	15224	1.48%	0.152%
16	10.522	1431	1434	1440	rVB	139713	118299	11.50%	1.181%
17	10.657	1453	1457	1466	rVB	30461	41666	4.05%	0.416%
18	11.098	1529	1532	1536	rBV3	33292	37509	3.65%	0.374%
19	11.216	1549	1552	1555	rBV	1059939	912382	88.67%	9.109%
20	11.239	1555	1556	1559	rVV	196228	110412	10.73%	1.102%
21	11.292	1560	1565	1568	rVB	32838	29389	2.86%	0.293%
22	11.445	1587	1591	1594	rBV2	16145	14718	1.43%	0.147%
23	11.527	1599	1605	1607	rBV	31286	24711	2.40%	0.247%
24	11.621	1618	1621	1625	rVB	227198	187325	18.21%	1.870%
25	11.716	1634	1637	1640	rBV	20944	18190	1.77%	0.182%
26	11.745	1640	1642	1647	rVB	28928	27523	2.67%	0.275%
27	11.827	1653	1656	1658	rBV	39225	39573	3.85%	0.395%
28	11.851	1658	1660	1666	rVB2	16721	14820	1.44%	0.148%
29	11.933	1671	1674	1679	rVB2	27049	25571	2.49%	0.255%
30	12.033	1689	1691	1695	rVB2	16316	15130	1.47%	0.151%
31	12.269	1727	1731	1733	rBV	20057	20896	2.03%	0.209%
32	12.304	1734	1737	1739	rVV	626532	525669	51.09%	5.248%
33	12.327	1739	1741	1743	rVV	565160	454127	44.14%	4.534%
34	12.345	1743	1744	1749	rVB3	51471	37869	3.68%	0.378%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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	12.421	1753	1757	1761	rVV2	227172	269263	26.17%	2.688%
36	12.468	1761	1765	1772	rVB7	5706	16423	1.60%	0.164%
37	12.651	1790	1796	1799	rBV	193606	189300	18.40%	1.890%
38	12.692	1799	1803	1805	rVB3	18442	20503	1.99%	0.205%
39	12.792	1818	1820	1828	rVB	241201	228160	22.17%	2.278%
40	12.874	1828	1834	1835	rBV3	13646	19867	1.93%	0.198%
41	12.980	1849	1852	1856	rVB	29934	28536	2.77%	0.285%
42	13.045	1860	1863	1866	rBV2	39780	34782	3.38%	0.347%
43	13.080	1866	1869	1872	rBV	19645	19344	1.88%	0.193%
44	13.174	1882	1885	1887	rBV	19061	16255	1.58%	0.162%
45	13.204	1887	1890	1894	rBV2	16860	20155	1.96%	0.201%
46	13.245	1894	1897	1901	rBV6	14614	18028	1.75%	0.180%
47	13.386	1918	1921	1926	rVB4	20756	22463	2.18%	0.224%
48	13.486	1936	1938	1942	rVB2	11380	13506	1.31%	0.135%
49	13.551	1946	1949	1953	rBV4	13080	14626	1.42%	0.146%
50	13.592	1953	1956	1959	rBV3	20084	30382	2.95%	0.303%
51	13.710	1974	1976	1981	rVB4	22408	24754	2.41%	0.247%
52	13.845	1994	1999	2002	rBV	1010384	952626	92.59%	9.511%
53	13.868	2002	2003	2006	rVB	88739	46295	4.50%	0.462%
54	14.027	2027	2030	2033	rVB2	27276	25764	2.50%	0.257%
55	14.327	2078	2081	2084	rBV3	35787	39904	3.88%	0.398%
56	14.621	2129	2131	2138	rVB	50755	72843	7.08%	0.727%
57	14.851	2167	2170	2179	rVB	76937	152018	14.77%	1.518%
58	14.939	2183	2185	2189	rVB2	61196	71008	6.90%	0.709%
59	15.133	2215	2218	2223	rBV	44035	48826	4.75%	0.487%
60	15.186	2224	2227	2232	rBV	58858	67719	6.58%	0.676%
61	15.251	2233	2238	2241	rBV	577674	645596	62.75%	6.446%
62	15.698	2310	2314	2319	rBV	62517	92264	8.97%	0.921%
63	16.156	2390	2392	2399	rVB3	52108	74830	7.27%	0.747%

Sum of corrected areas: 10015833

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Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
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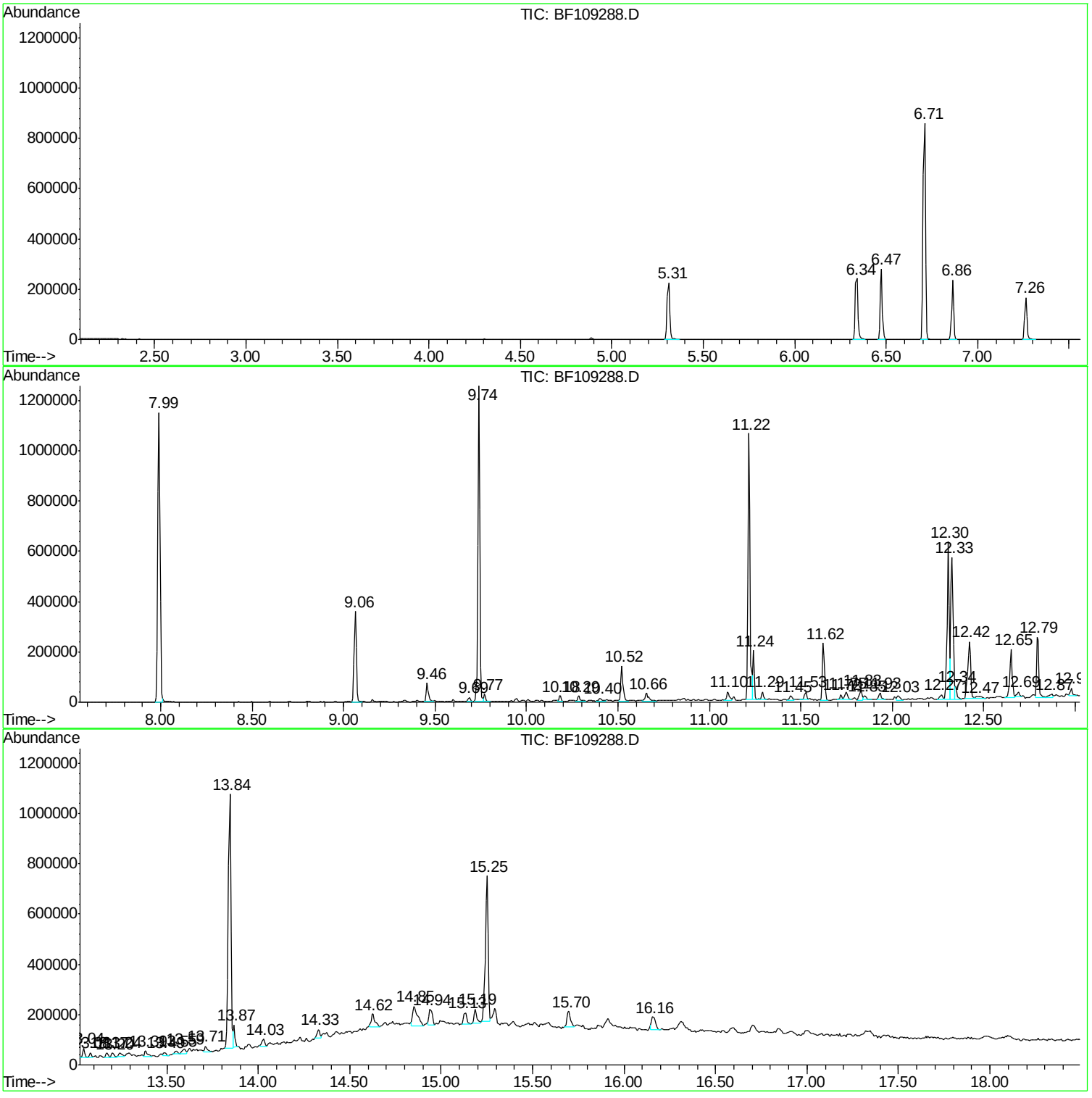
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-03-092418

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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

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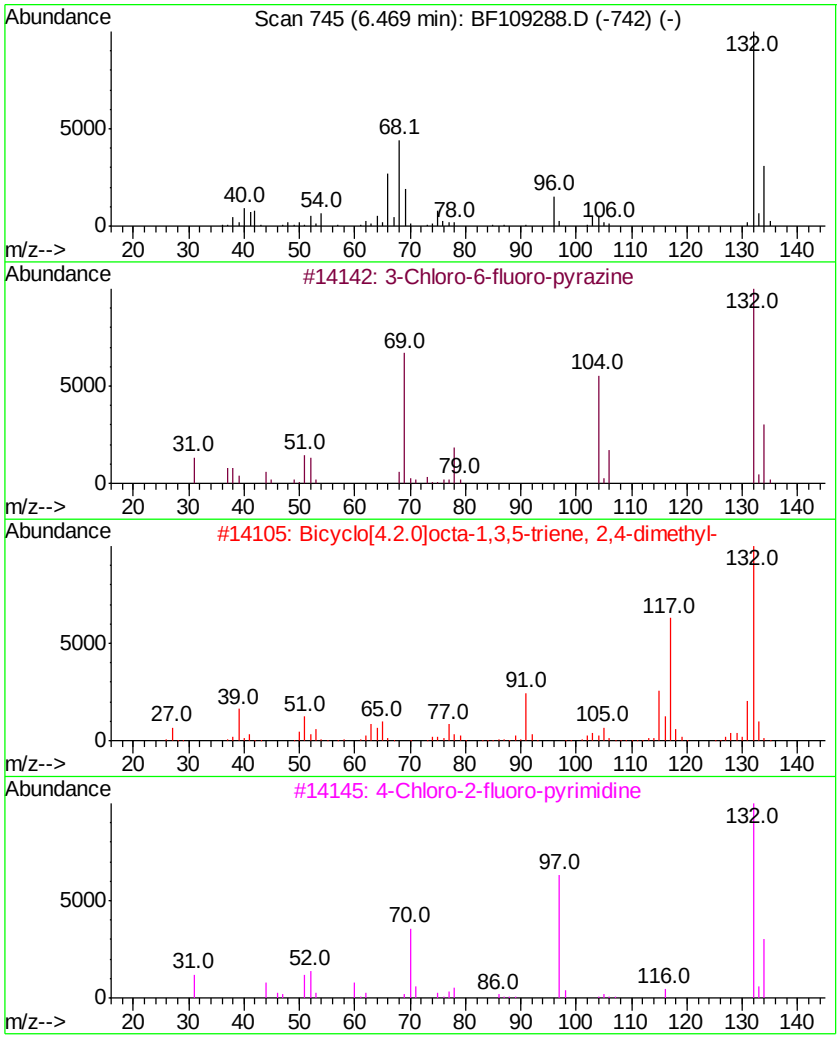
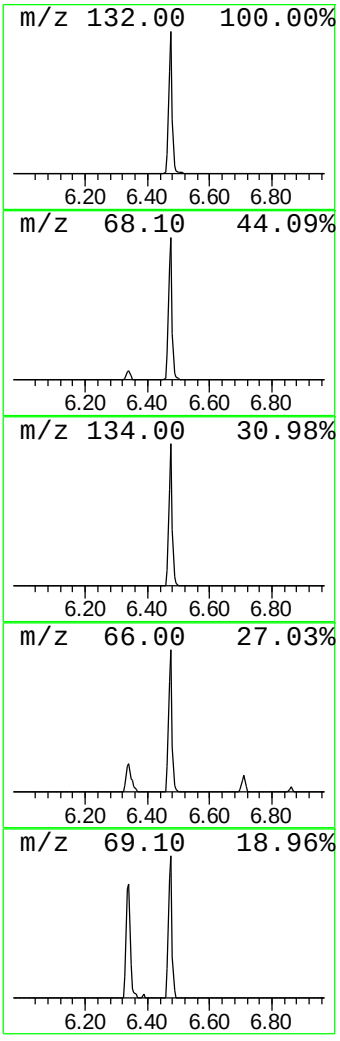
Peak Number 1 unknown6.47 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	6.43 ng	228919	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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

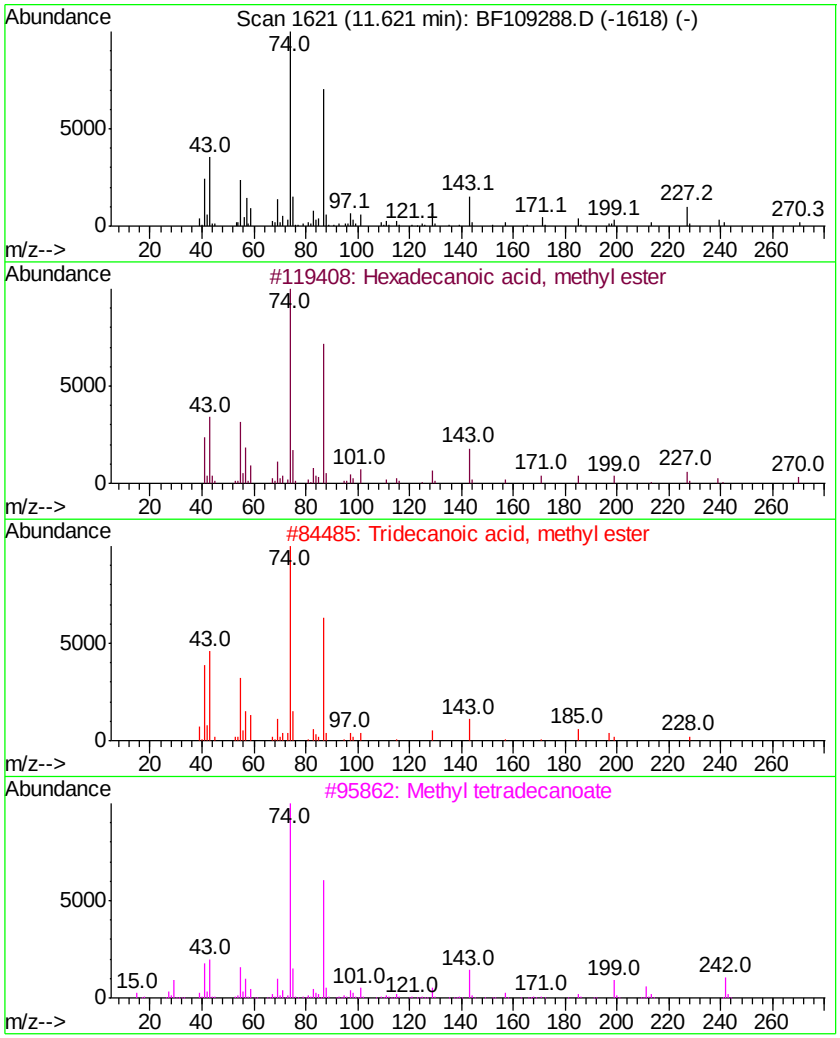
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

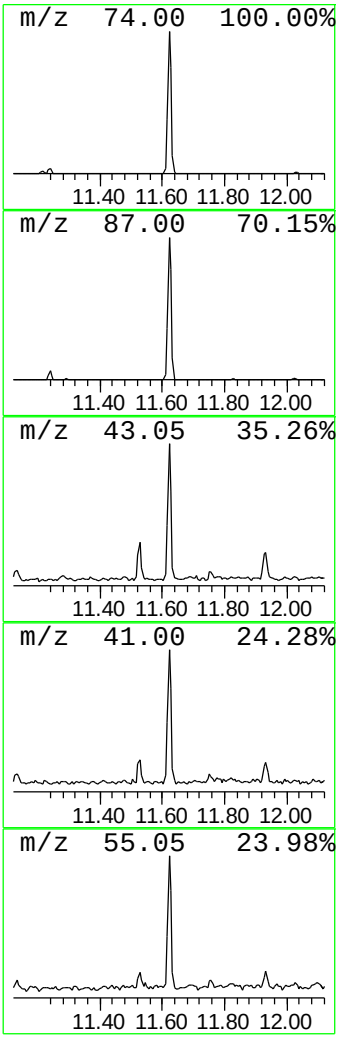
****

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	4.11 ng	187325	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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

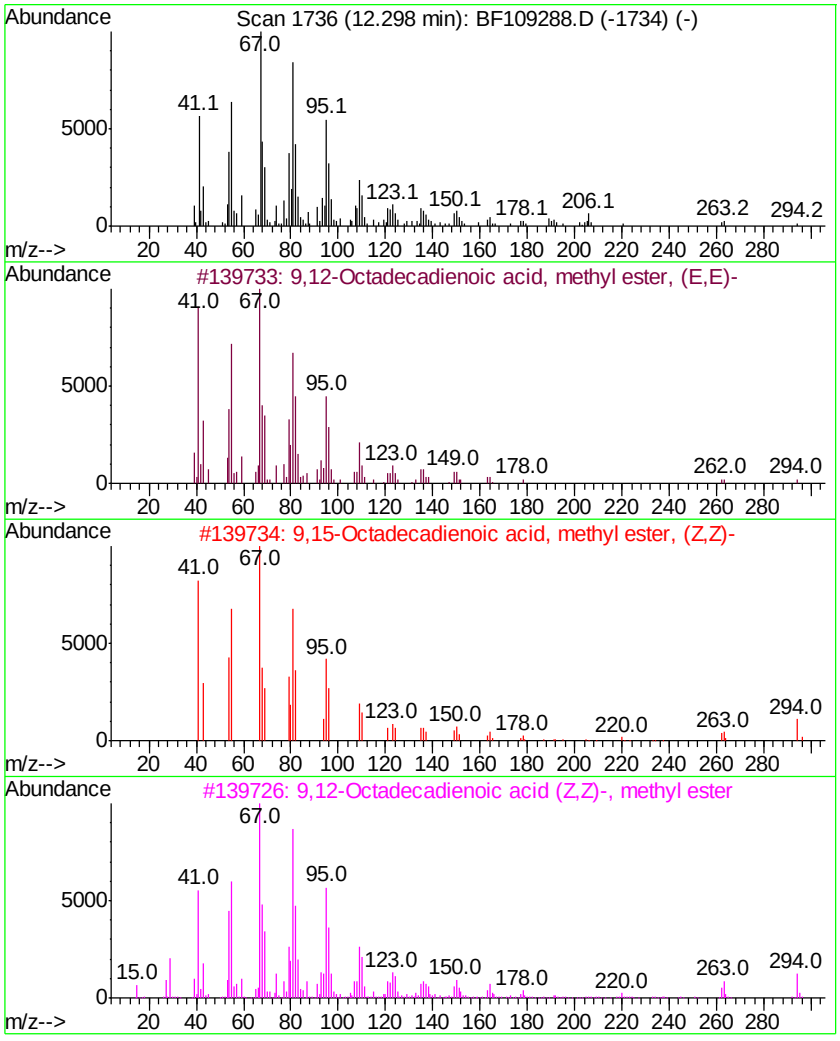
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

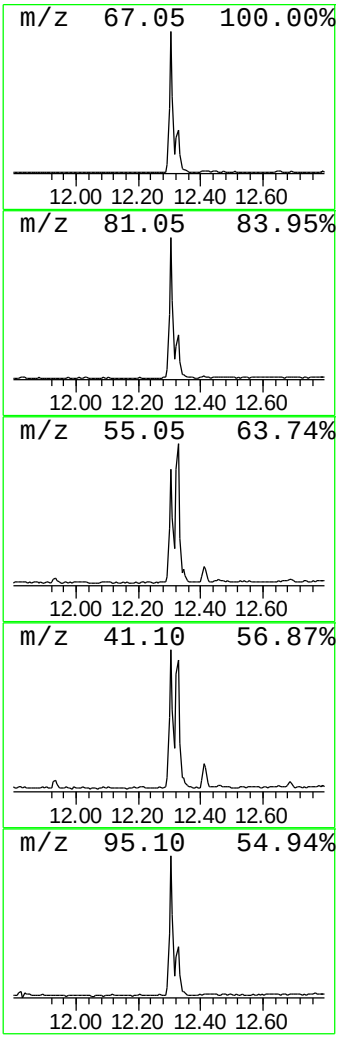
****

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	11.52 ng	525669	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 (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	97
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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

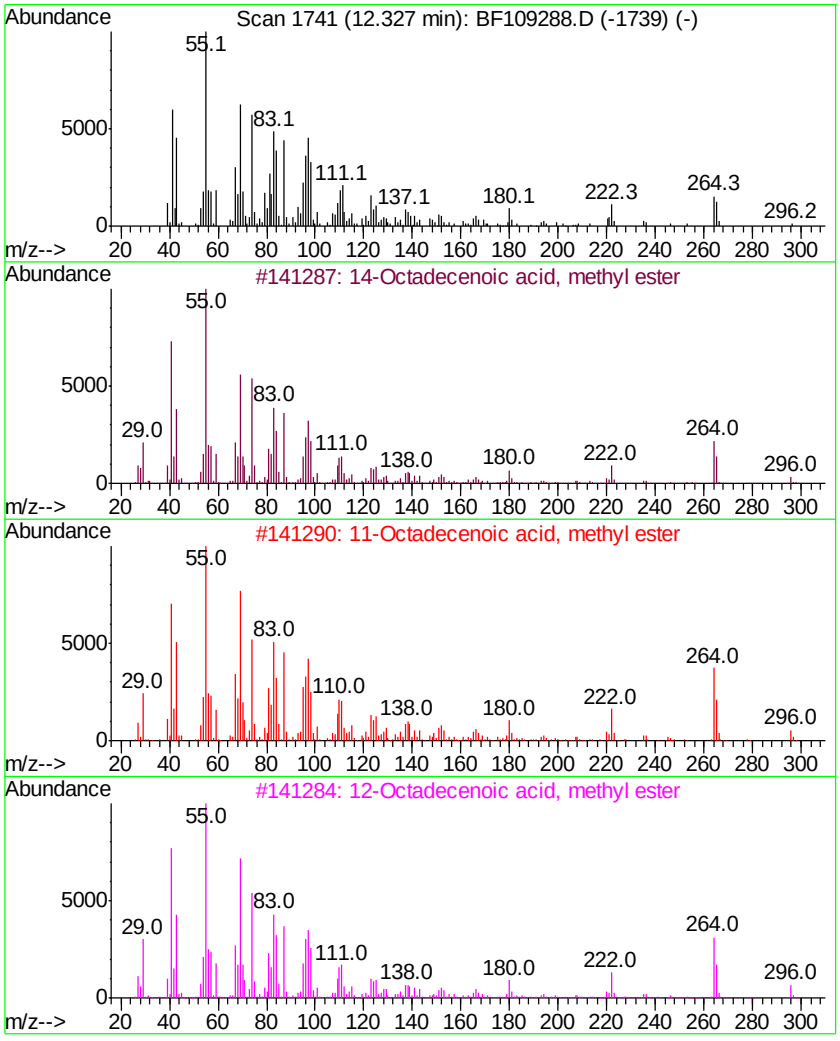
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

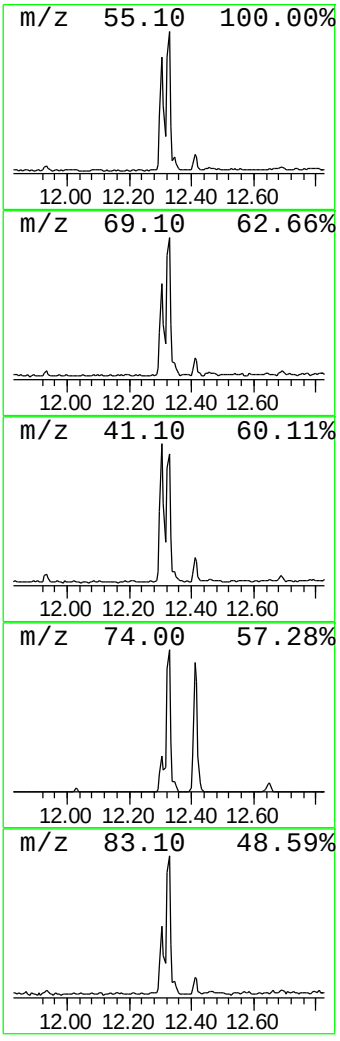
****

Peak Number 5 14-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	9.95 ng	454127	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
3	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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

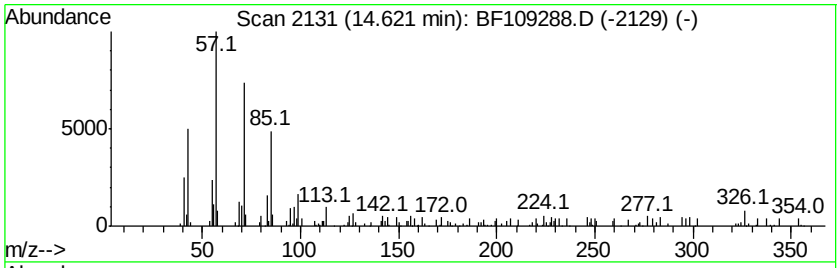
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

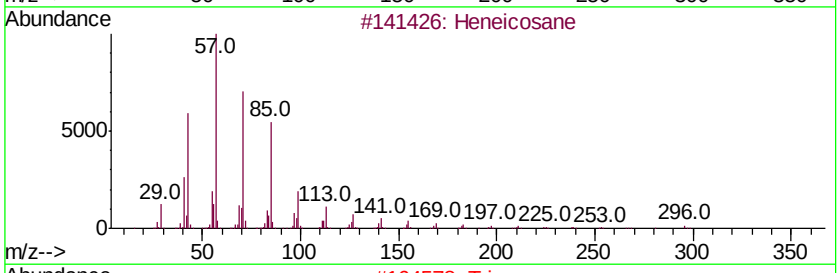
****

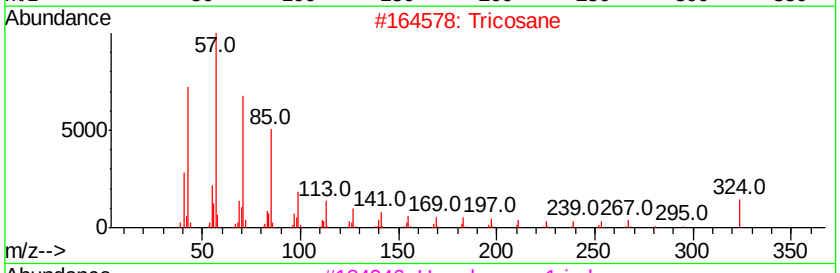
Peak Number 6 Heneicosane Concentration Rank 8

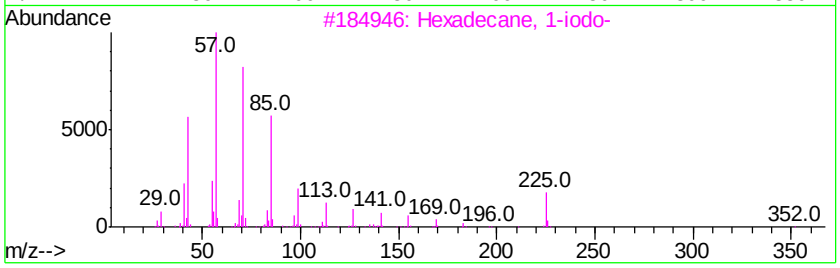
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.26 ng	72843	Perylene-d12	15.25

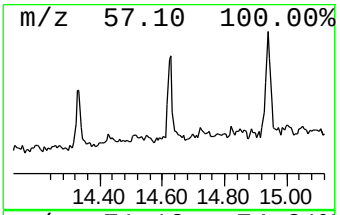
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	89
2	Tricosane	324	C23H48	000638-67-5	76
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	64
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
5	Heptadecane	240	C17H36	000629-78-7	64

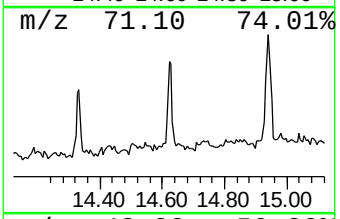


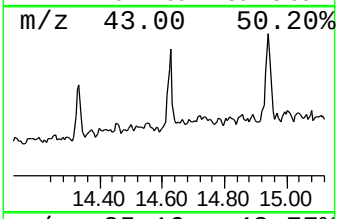


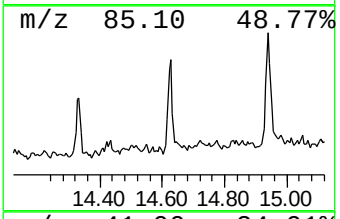


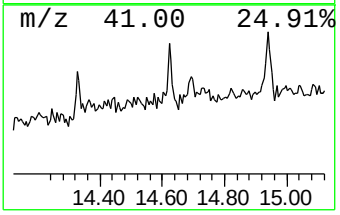












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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

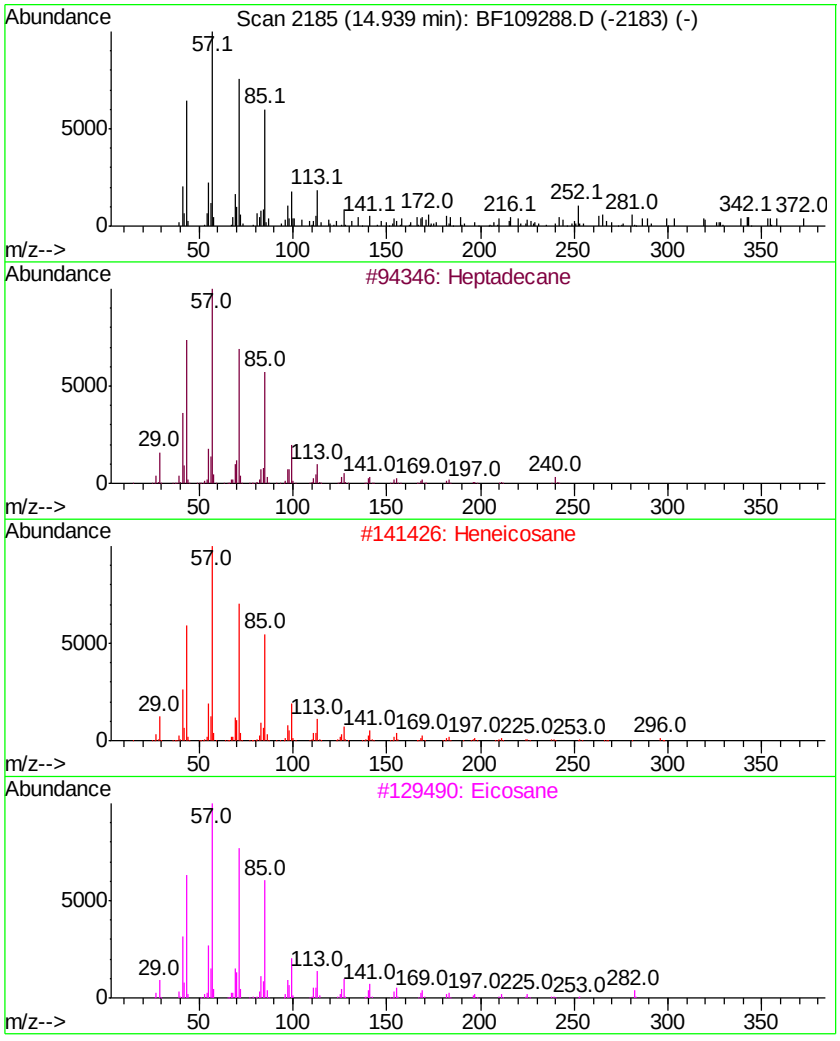
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

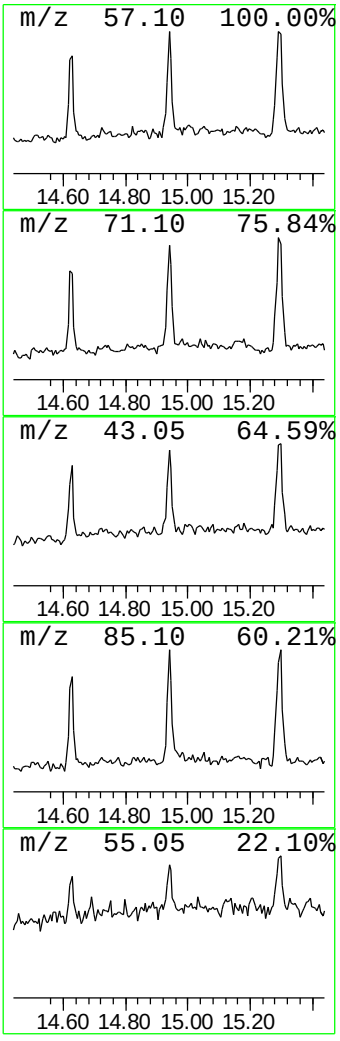
****

Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	2.20 ng	71008	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Heneicosane	296	C21H44	000629-94-7	70
3	Eicosane	282	C20H42	000112-95-8	62
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	62
5	Octadecane	254	C18H38	000593-45-3	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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

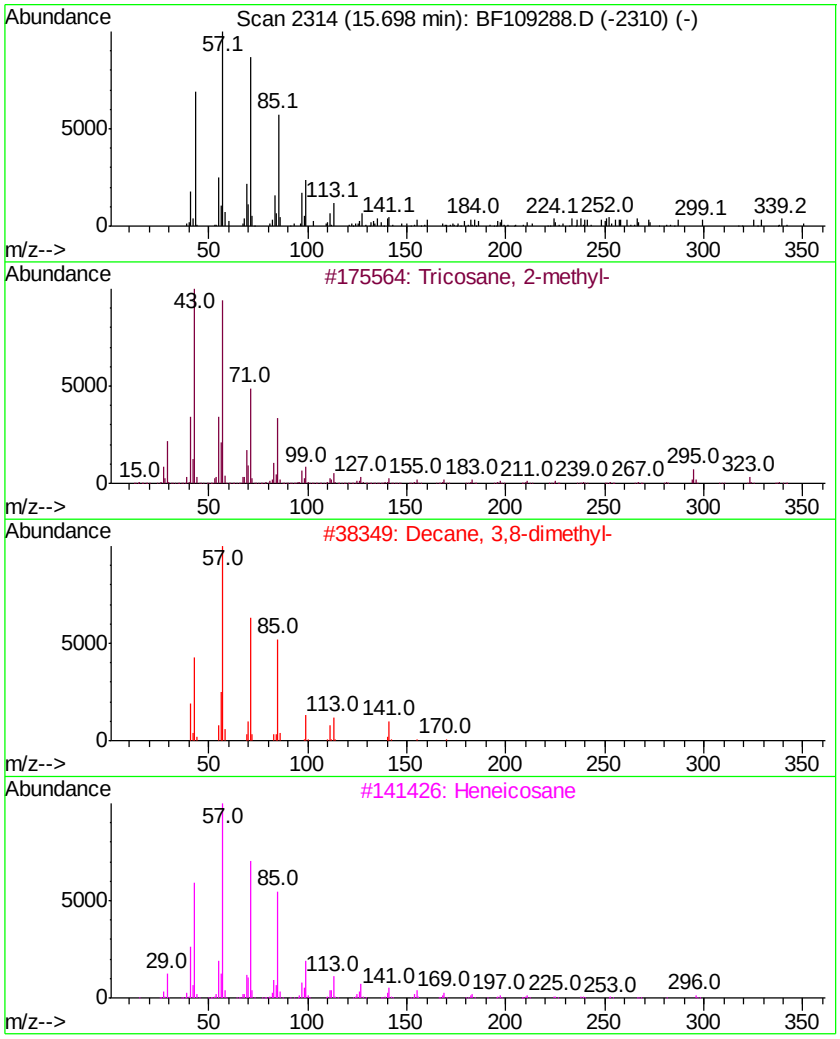
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

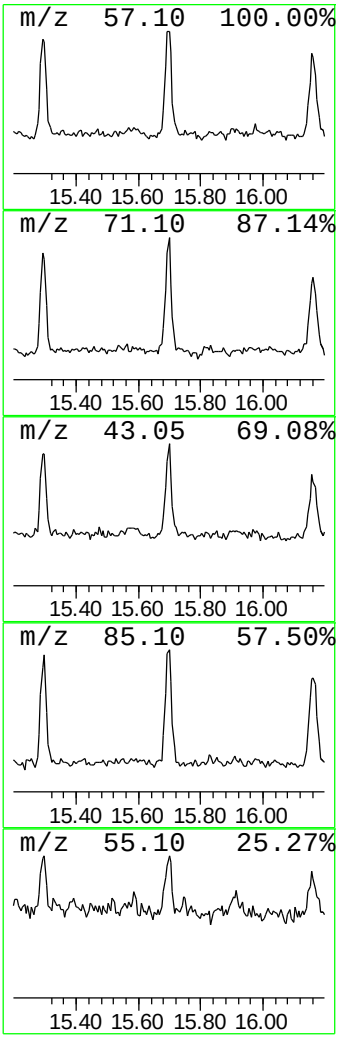
****

Peak Number 8 Tricosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.86 ng	92264	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane, 2-methyl-	338	C24H50	001928-30-9	89
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	76
3	Heneicosane	296	C21H44	000629-94-7	74
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	72
5	Pentacosane	352	C25H52	000629-99-2	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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

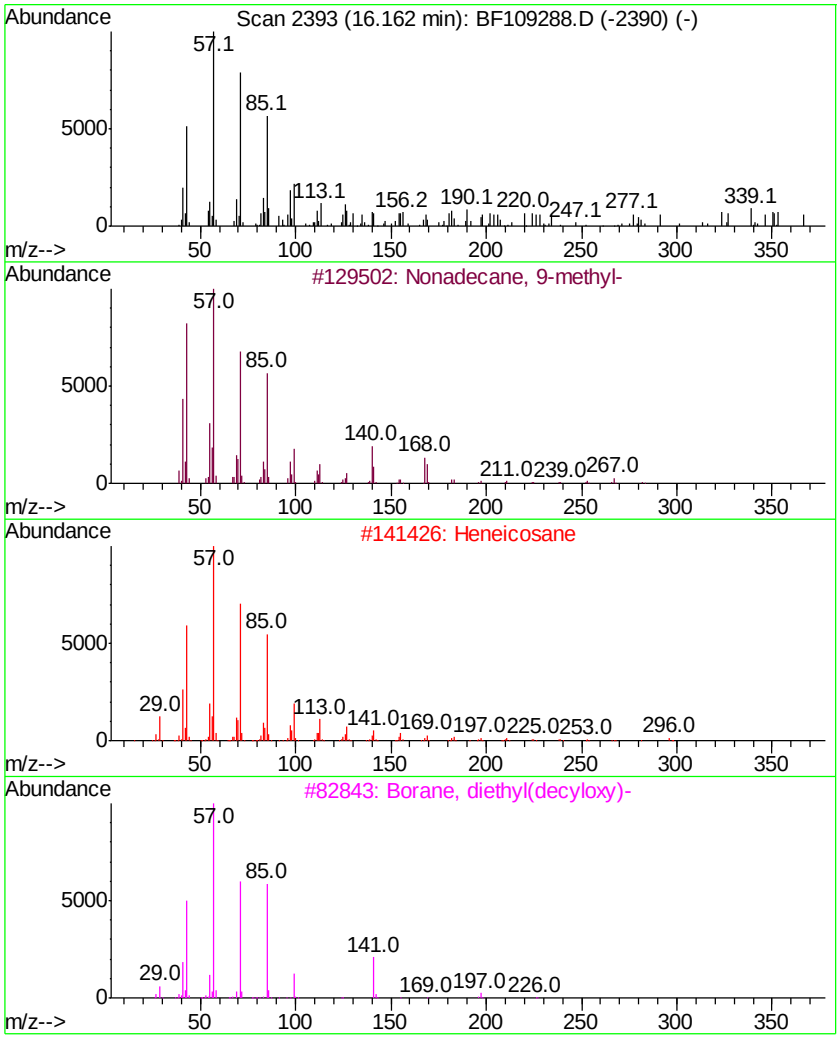
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

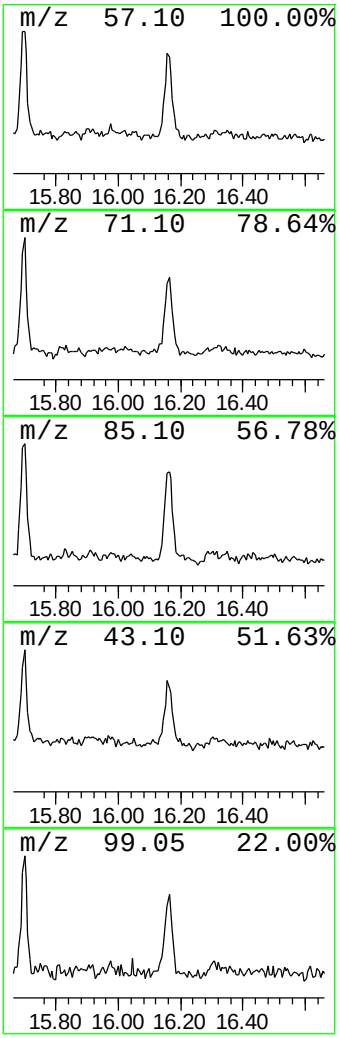
****

Peak Number 9 Nonadecane, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	2.32 ng	74830	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	52
2	Heneicosane	296	C21H44	000629-94-7	52
3	Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	50
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	50
5	Eicosane	282	C20H42	000112-95-8	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092518\
Data File : BF109288.D
Acq On : 25 Sep 2018 16:25
Operator : JU/SJ
Sample : J4774-05 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-092418

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
unknown6.47	6.47	6.4	ng	228919	1	6.71	712436	20.0
Hexadecanoic acid...	11.62	4.1	ng	187325	4	11.22	912382	20.0
9,12-Octadecadien...	12.30	11.5	ng	525669	4	11.22	912382	20.0
14-Octadecenoic a...	12.33	9.9	ng	454127	4	11.22	912382	20.0
Heneicosane	14.62	2.3	ng	72843	6	15.25	645596	20.0
Heptadecane	14.94	2.2	ng	71008	6	15.25	645596	20.0
Tricosane, 2-methyl-	15.70	2.9	ng	92264	6	15.25	645596	20.0
Nonadecane, 9-met...	16.16	2.3	ng	74830	6	15.25	645596	20.0