LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112804.D
Acq On : 1 Mar 2019 17:16
Operator : JU/SJ
Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

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-BF022719.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	5.346	550	554	568	rBV	1723552	1646421	88.47%	5.819%
2	6.369	724	728	741	rBV	1965985	1801566	96.81%	6.367%
3	6.510	748	752	755	rBV	1960779	1748929	93.98%	6.181%
4	6.745	788	792	795	rBV	1075462	992062	53.31%	3.506%
5	6.898	814	818	822	rBV	1624544	1334941	71.73%	4.718%
6	7.298	881	886	894	rBV	1139795	1040911	55.93%	3.679%
7	8.022	1005	1009	1016	rBV	1313193	1228470	66.01%	4.342%
8	8.463	1079	1084	1085	rBV2	26407	30406	1.63%	0.107%
9	8.628	1108	1112	1115	rBV	36412	37973	2.04%	0.134%
10	8.839	1145	1148	1155	rVB6	10921	22327	1.20%	0.079%
11	9.057	1182	1185	1188	rVB4	22123	19215	1.03%	0.068%
12	9.098	1188	1192	1203	rBV	1954668	1690330	90.83%	5.974%
13	9.192	1203	1208	1212	rVB4	51751	59650	3.21%	0.211%
14	9.486	1255	1258	1265	rBV	164169	177405	9.53%	0.627%
15	9.634	1279	1283	1291	rBV	133546	172397	9.26%	0.609%
16	9.692	1291	1293	1295	rVB	51632	37486	2.01%	0.132%
17	9.722	1295	1298	1302	rVB	37052	31611	1.70%	0.112%
18	9.775	1302	1307	1314	rBV	1157721	1162114	62.45%	4.107%
19	10.222	1379	1383	1388	rBV3	37047	37167	2.00%	0.131%
20	10.316	1397	1399	1406	rBV3	15508	23334	1.25%	0.082%
21	10.433	1413	1419	1423	rBV2	19526	31499	1.69%	0.111%
22	10.551	1435	1439	1450	rBV	932754	905565	48.66%	3.201%
23	10.686	1458	1462	1469	rVB3	38936	54958	2.95%	0.194%
24	11.133	1535	1538	1542	rBV3	27420	25971	1.40%	0.092%
25	11.251	1554	1558	1560	rBV	1068548	998523	53.66%	3.529%
26	11.269	1560	1561	1566	rVV	120483	97342	5.23%	0.344%
27	11.322	1566	1570	1574	rVV	59746	56655	3.04%	0.200%
28	11.657	1623	1627	1632	rVB	100306	89887	4.83%	0.318%
29	11.751	1640	1643	1645	rBV	30495	24702	1.33%	0.087%
30	11.786	1645	1649	1653	rBV2	227955	240425	12.92%	0.850%
31	11.822	1653	1655	1658	rVB2	34747	29692	1.60%	0.105%
32	11.857	1658	1661	1664	rBV	70672	75969	4.08%	0.269%
33	11.928	1670	1673	1677	rBV	63237	54377	2.92%	0.192%
34	12.045	1690	1693	1695	rBV	32736	30230	1.62%	0.107%

LSC Area Percent Report

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Data File : BF112804.D
Acq On : 1 Mar 2019 17:16
Operator : JU/SJ
Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.192	1713	1718	1720	rBV4	17890	26362	1.42%	0.093%
36	12.227	1720	1724	1725	rBV	20828	18922	1.02%	0.067%
37	12.298	1732	1736	1739	rBV2	70110	72333	3.89%	0.256%
38	12.339	1739	1743	1744	rVV2	283501	268726	14.44%	0.950%
39	12.357	1744	1746	1754	rVB2	559233	572516	30.76%	2.023%
40	12.457	1758	1763	1764	rBV	531534	520815	27.99%	1.841%
41	12.475	1764	1766	1767	rVV	299517	255155	13.71%	0.902%
42	12.492	1767	1769	1776	rVV2	336645	406872	21.86%	1.438%
43	12.551	1776	1779	1780	rVV	73073	74406	4.00%	0.263%
44	12.586	1780	1785	1787	rVV2	166873	231171	12.42%	0.817%
45	12.604	1787	1788	1796	rVB2	112882	112134	6.03%	0.396%
46	12.680	1796	1801	1805	rBV	623979	610584	32.81%	2.158%
47	12.804	1819	1822	1823	rBV	39911	36407	1.96%	0.129%
48	12.827	1823	1826	1833	rVB	1656790	1451372	77.99%	5.130%
49	12.904	1833	1839	1846	rBV4	84632	149135	8.01%	0.527%
50	12.986	1850	1853	1854	rVV2	73327	68686	3.69%	0.243%
51	13.010	1854	1857	1860	rVB2	141736	142220	7.64%	0.503%
52	13.045	1860	1863	1865	rBV4	16404	19600	1.05%	0.069%
53	13.074	1865	1868	1871	rVV	105107	95032	5.11%	0.336%
54	13.110	1871	1874	1878	rVV	116324	119177	6.40%	0.421%
55	13.174	1882	1885	1887	rBV2	36690	40496	2.18%	0.143%
56	13.204	1887	1890	1893	rVV	76395	61266	3.29%	0.217%
57	13.233	1893	1895	1900	rVV2	63986	62001	3.33%	0.219%
58	13.416	1923	1926	1931	rVB3	59471	82942	4.46%	0.293%
59	13.510	1940	1942	1948	rVB	77534	97017	5.21%	0.343%
60	13.574	1951	1953	1955	rBV	25847	19124	1.03%	0.068%
61	13.622	1957	1961	1964	rBV3	89106	119714	6.43%	0.423%
62	13.651	1964	1966	1968	rVV	70066	64032	3.44%	0.226%
63	13.674	1968	1970	1974	rVV2	83561	110167	5.92%	0.389%
64	13.733	1975	1980	1988	rVB3	148000	241046	12.95%	0.852%
65	13.874	1999	2004	2007	rBV2	1551701	1860960	100.00%	6.577%
66	13.898	2007	2008	2011	rVB	439599	259214	13.93%	0.916%
67	14.016	2026	2028	2030	rBV	51401	35649	1.92%	0.126%
68	14.057	2033	2035	2038	rVB2	88813	78702	4.23%	0.278%
69	14.086	2038	2040	2045	rBV2	38324	51782	2.78%	0.183%
70	14.257	2067	2069	2072	rVB	127709	124980	6.72%	0.442%
71	14.292	2073	2075	2078	rVB	85773	69767	3.75%	0.247%

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Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

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

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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.363	2083	2087	2089	rVV3	128616	181016	9.73%	0.640%
73	14.404	2092	2094	2099	rVB3	81826	80134	4.31%	0.283%
74	14.663	2135	2138	2144	rVB2	129943	160350	8.62%	0.567%
75	14.886	2172	2176	2179	rBV	480135	759838	40.83%	2.686%
76	14.980	2189	2192	2199	rVB2	239113	289299	15.55%	1.022%
77	15.168	2220	2224	2229	rVB	254456	307678	16.53%	1.087%
78	15.221	2230	2233	2238	rVB	367610	433452	23.29%	1.532%
79	15.286	2239	2244	2247	rBV	829266	987202	53.05%	3.489%
80	16.639	2471	2474	2483	rVB2	155879	283425	15.23%	1.002%
81	17.045	2540	2543	2551	rVB	99282	170197	9.15%	0.602%

Sum of corrected areas: 28293585

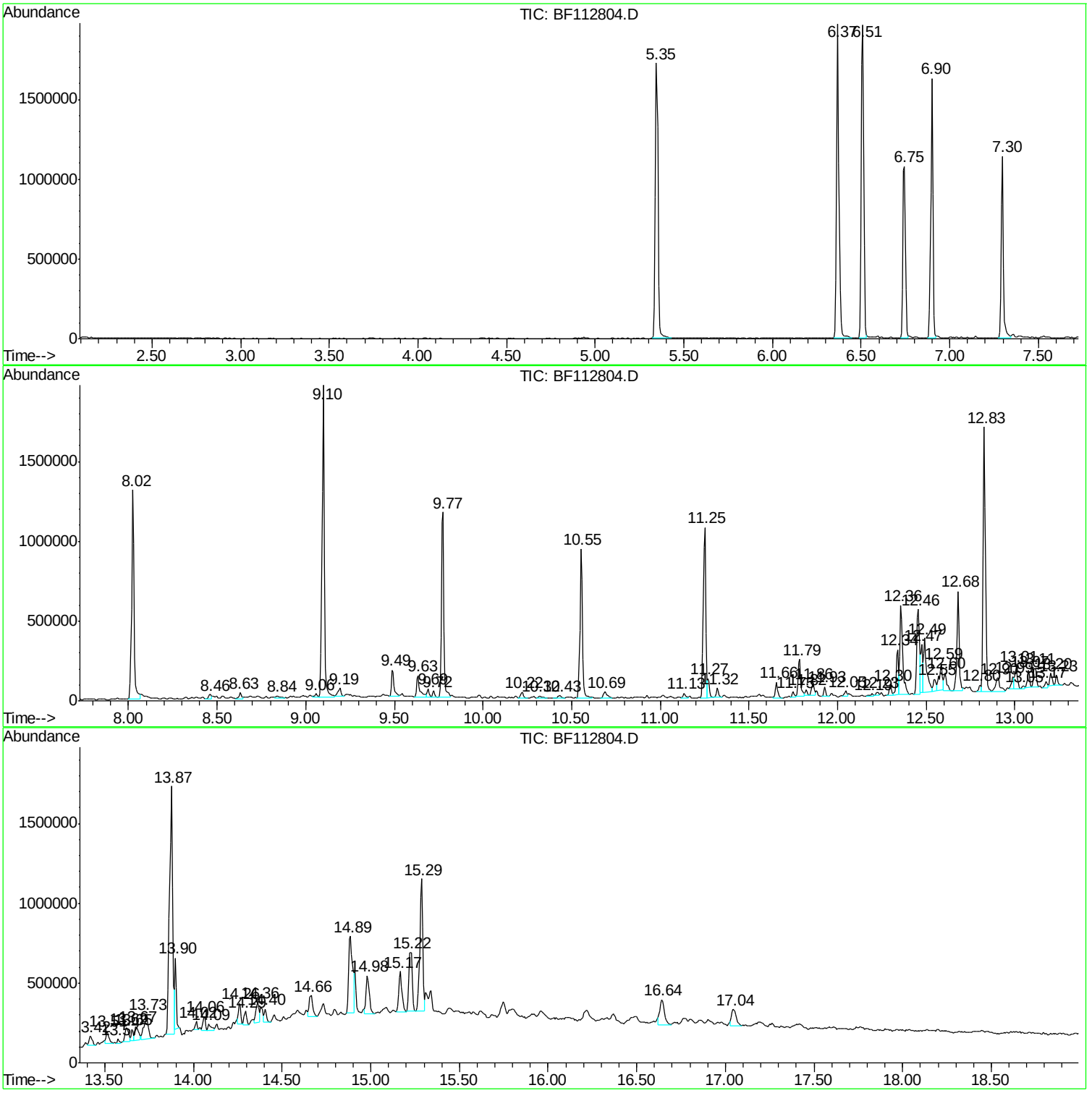
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112804.D
Acq On : 1 Mar 2019 17:16
Operator : JU/SJ
Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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\BF030119\
Data File : BF112804.D
Acq On : 1 Mar 2019 17:16
Operator : JU/SJ
Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

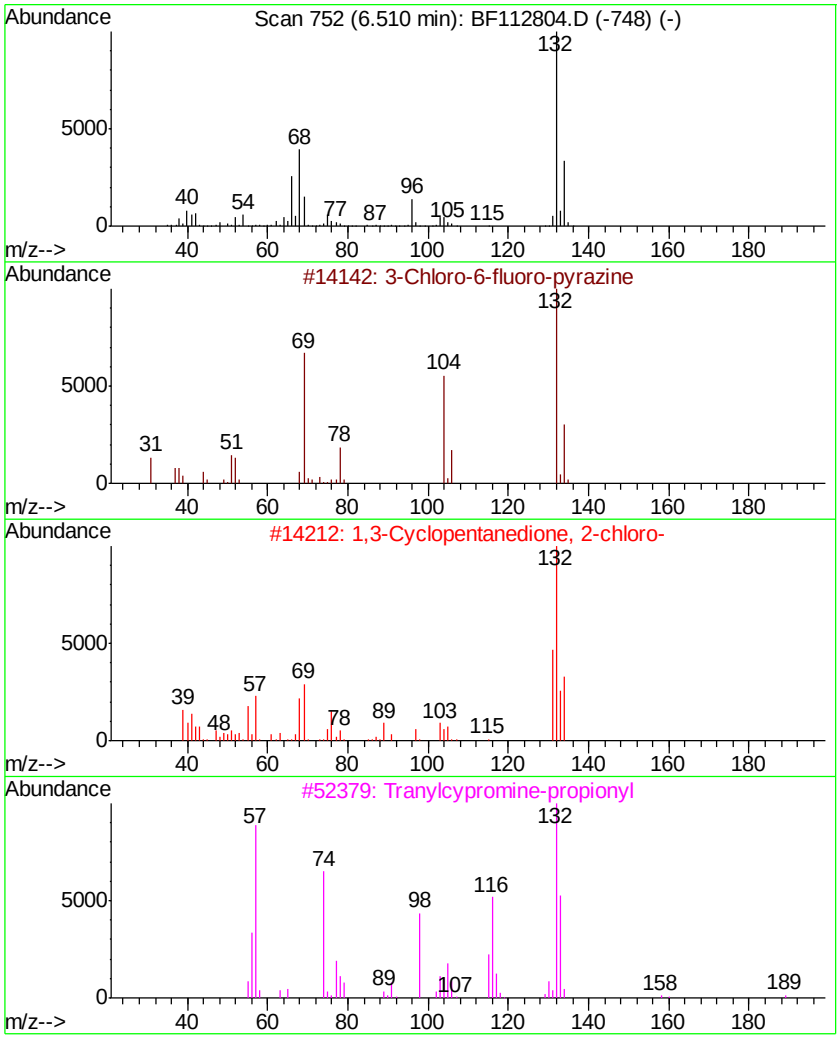
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

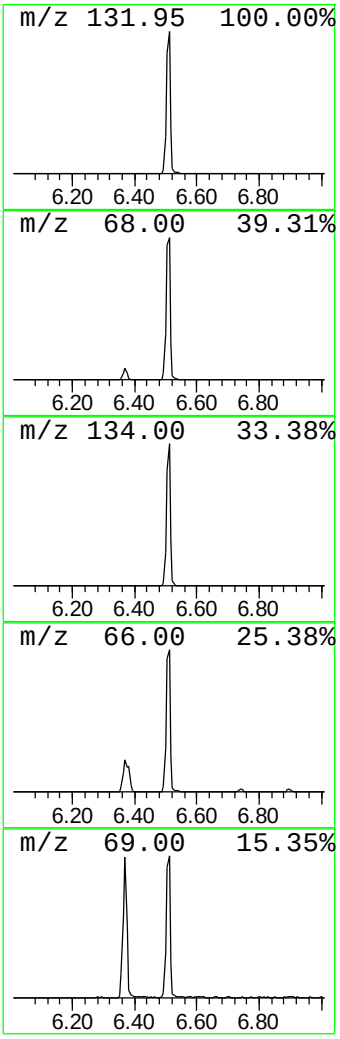
****

Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	35.26 ng	1748930	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
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\BF030119\
Data File : BF112804.D
Acq On : 1 Mar 2019 17:16
Operator : JU/SJ
Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

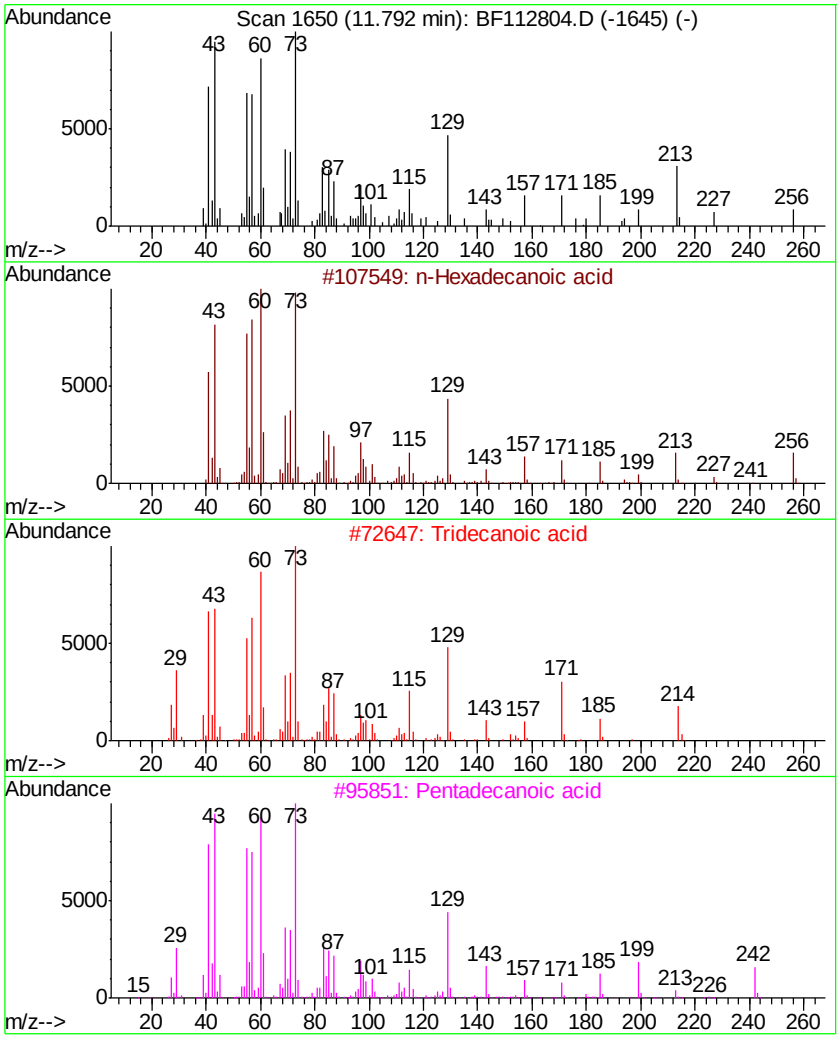
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

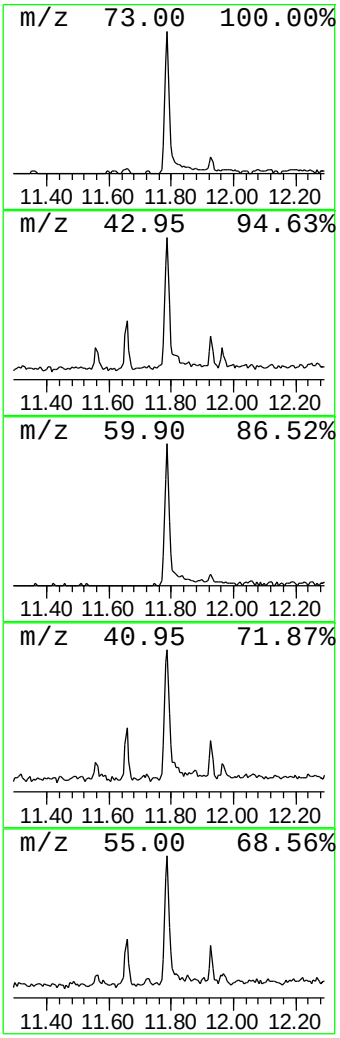
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	4.82 ng	240425	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

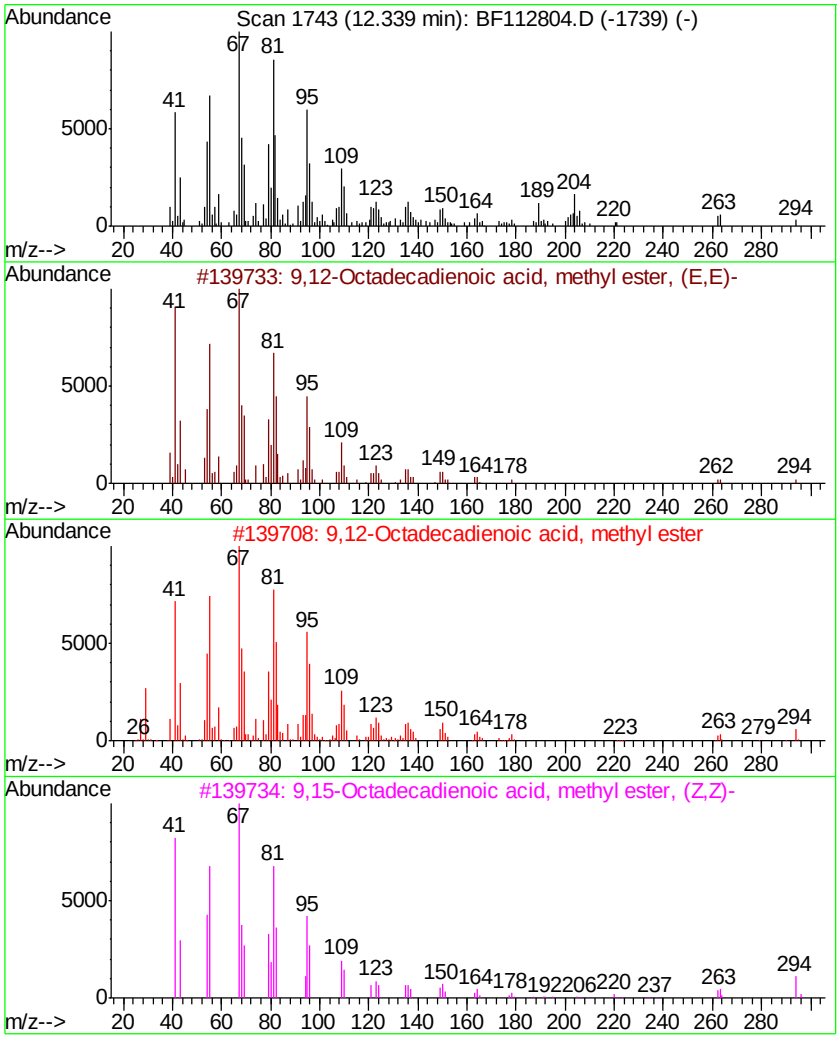
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

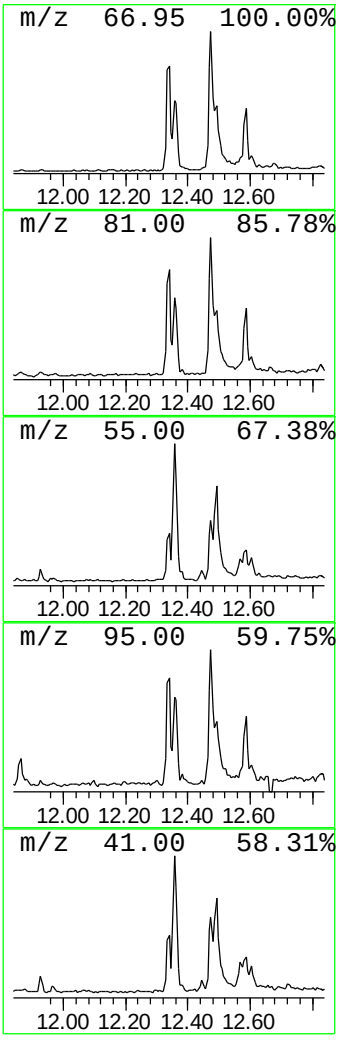
****

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	5.38 ng	268726	Phenanthrene-d10	11.25

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, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	94





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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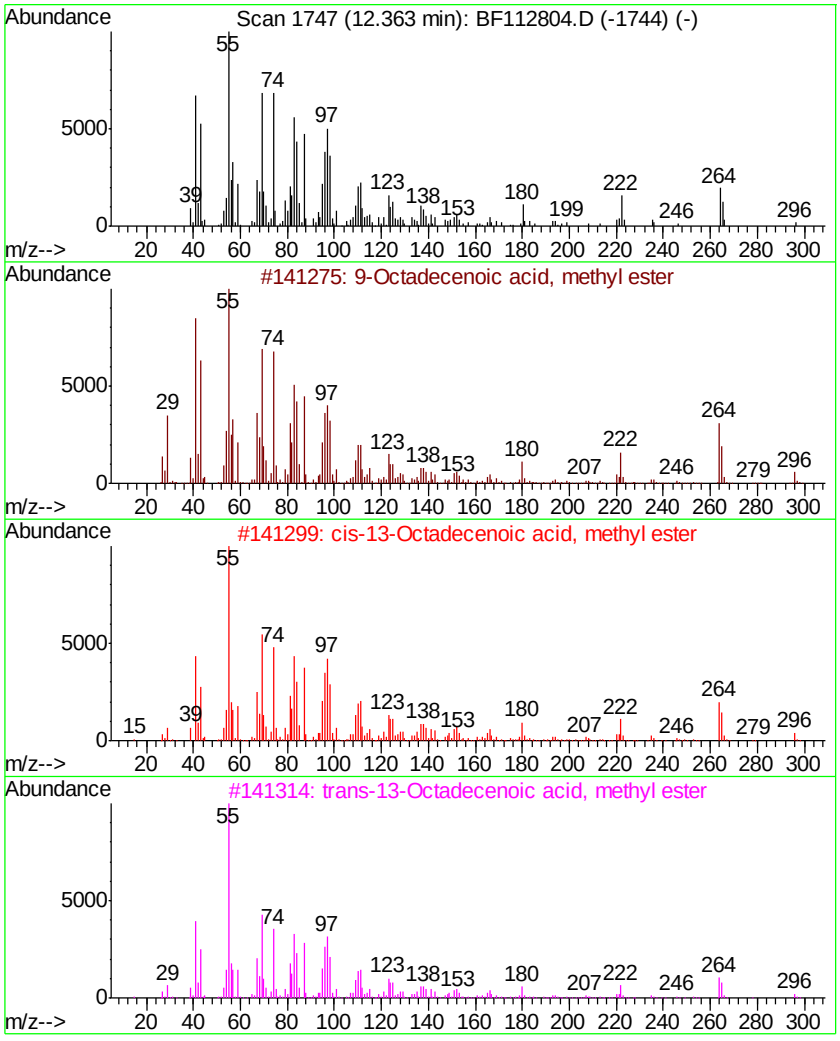
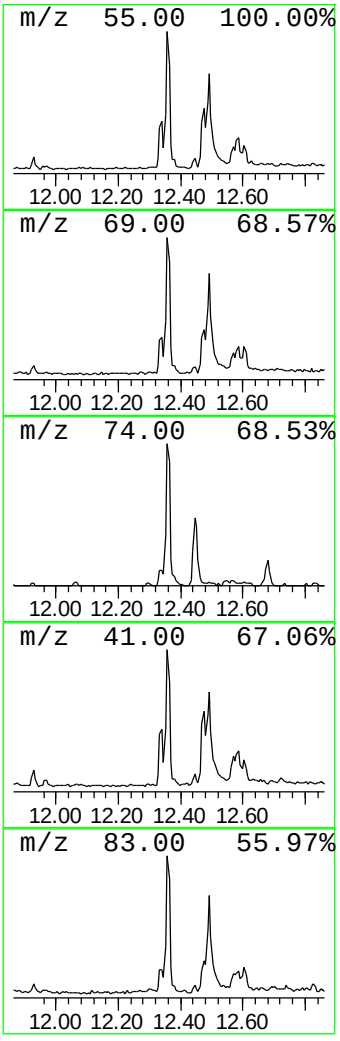
Peak Number 5 9-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	11.47 ng	572516	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	98
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	97
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	97
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	96





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Operator : JU/SJ
Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

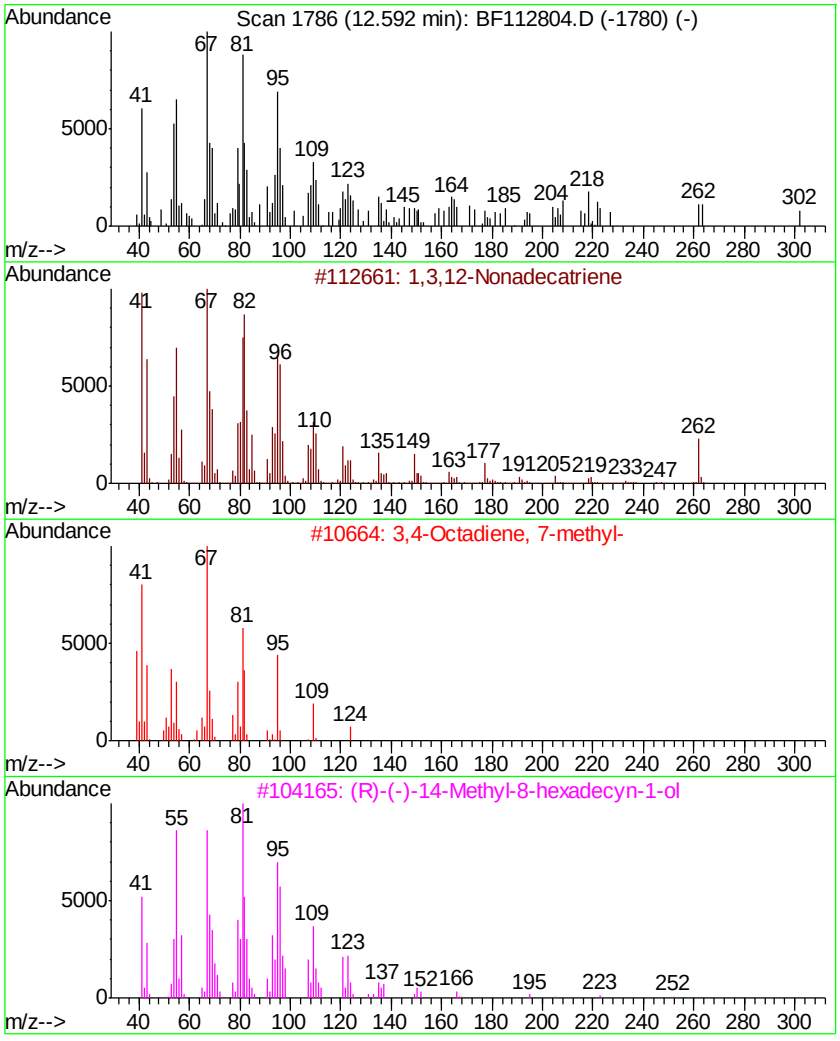
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

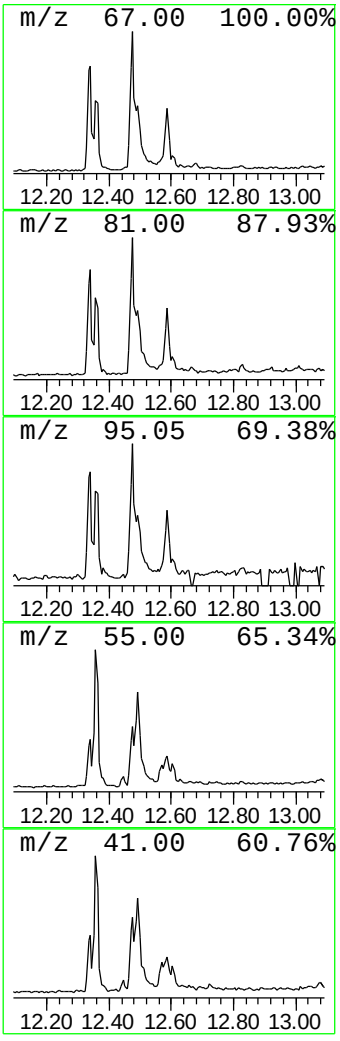
****

Peak Number 6 1,3,12-Nonadecatriene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	2.48 ng	231171	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,12-Nonadecatriene	262	C19H34	1000131-11-1	83
2	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	76
3	(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	064566-18-3	74
4	8-Hexadecyne	222	C16H30	019781-86-3	72
5	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
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Acq On : 1 Mar 2019 17:16
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Sample : K1670-03 2X
Misc :
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Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

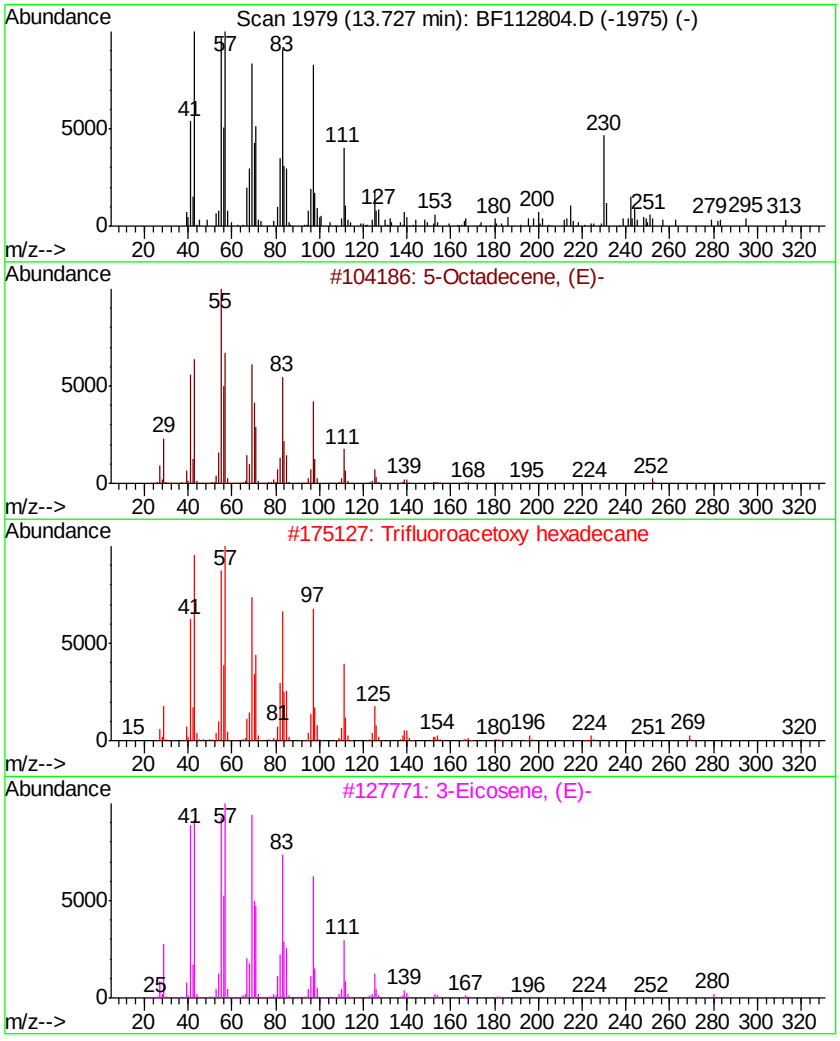
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

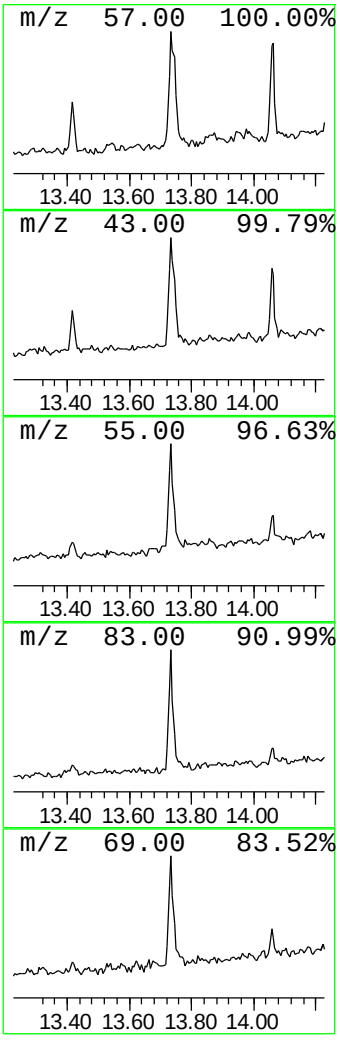
****

Peak Number 7 5-Octadecene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.59 ng	241046	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
5	1-Octadecene	252	C18H36	000112-88-9	92





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112804.D
Acq On : 1 Mar 2019 17:16
Operator : JU/SJ
Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

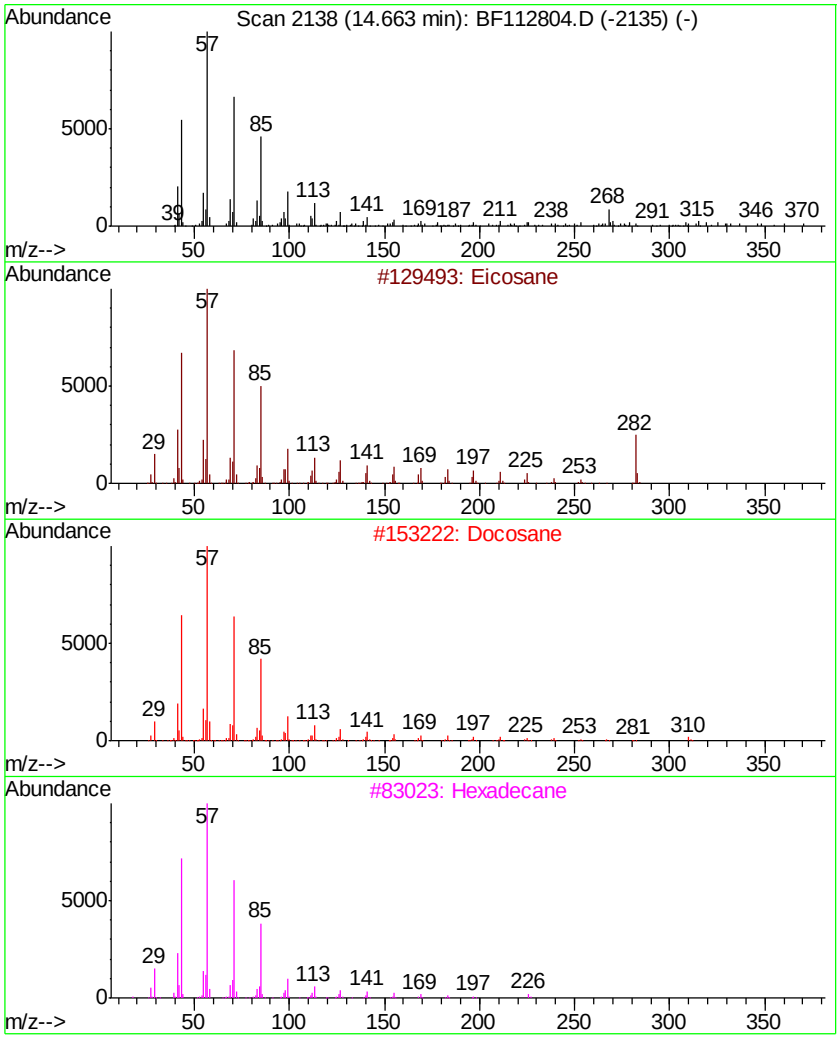
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

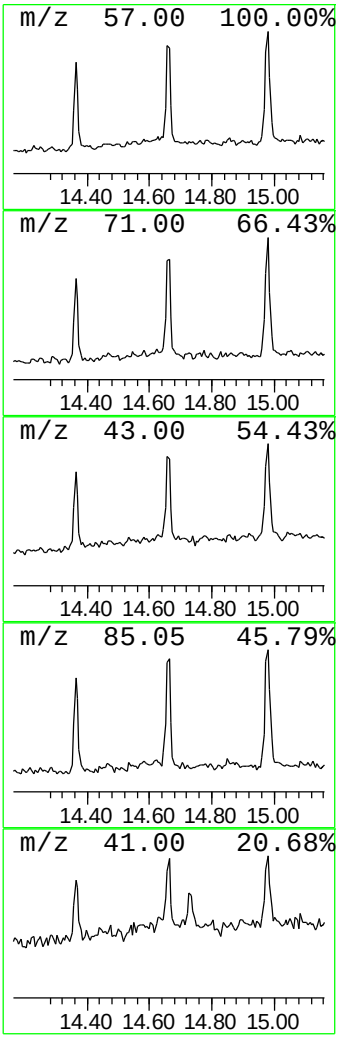
****

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.25 ng	160350	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Docosane	310	C22H46	000629-97-0	93
3	Hexadecane	226	C16H34	000544-76-3	87
4	Nonadecane	268	C19H40	000629-92-5	86
5	Triacontane	422	C30H62	000638-68-6	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030119\
Data File : BF112804.D
Acq On : 1 Mar 2019 17:16
Operator : JU/SJ
Sample : K1670-03 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-032-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.51	6.51	35.3	ng	1748930	1	6.75	992062	20.0
n-Hexadecanoic acid	11.79	4.8	ng	240425	4	11.25	998523	20.0
9,12-Octadecadien...	12.34	5.4	ng	268726	4	11.25	998523	20.0
9-Octadecenoic ac...	12.36	11.5	ng	572516	4	11.25	998523	20.0
1,3,12-Nonadecatr...	12.59	2.5	ng	231171	5	13.87	1860960	20.0
5-Octadecene, (E)-	13.73	2.6	ng	241046	5	13.87	1860960	20.0
Eicosane	14.66	3.3	ng	160350	6	15.29	987202	20.0