LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

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-BF083018.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	5.242	491	494	504	rBV	22016	38715	1.97%	0.199%
2	5.648	559	563	586	rBV	233611	982584	50.08%	5.051%
3	6.642	728	732	751	rBV	451615	1373649	70.01%	7.061%
4	6.772	751	754	779	rVB	873605	1651489	84.18%	8.490%
5	7.001	789	793	815	rVB	264432	535924	27.32%	2.755%
6	7.154	815	819	847	rVB	822649	1220685	62.22%	6.275%
7	7.566	885	889	915	rBV	463857	1025200	52.25%	5.270%
8	8.283	1007	1011	1038	rBV	408228	724686	36.94%	3.725%
9	9.348	1189	1192	1215	rBV	1551473	1961949	100.00%	10.086%
10	9.748	1256	1260	1272	rBV	89734	119624	6.10%	0.615%
11	10.042	1306	1310	1329	rBV	708354	844908	43.06%	4.343%
12	10.419	1371	1374	1381	rBV	75705	75095	3.83%	0.386%
13	10.836	1441	1445	1456	rBV	922566	1242674	63.34%	6.388%
14	11.536	1561	1564	1577	rBV	729596	902579	46.00%	4.640%
15	12.042	1646	1650	1653	rBV2	38898	54301	2.77%	0.279%
16	12.077	1653	1656	1660	rVB	21600	28762	1.47%	0.148%
17	12.760	1769	1772	1777	rBV	66420	74459	3.80%	0.383%
18	12.971	1804	1808	1809	rBV4	26144	32222	1.64%	0.166%
19	12.989	1809	1811	1815	rVB	68826	78026	3.98%	0.401%
20	13.077	1823	1826	1829	rBV3	16059	25157	1.28%	0.129%
21	13.118	1829	1833	1845	rVV	1859789	1837260	93.64%	9.445%
22	13.318	1865	1867	1870	rBV2	25956	20560	1.05%	0.106%
23	13.630	1917	1920	1923	rBV	137146	122146	6.23%	0.628%
24	13.665	1923	1926	1928	rVB	27548	28268	1.44%	0.145%
25	13.989	1979	1981	1983	rBV2	29385	27682	1.41%	0.142%
26	14.189	2011	2015	2028	rBV	664484	859825	43.83%	4.420%
27	14.307	2032	2035	2038	rBV	76682	81017	4.13%	0.416%
28	14.413	2050	2053	2057	rBV2	55505	68641	3.50%	0.353%
29	14.612	2082	2087	2091	rBV	192828	259188	13.21%	1.332%
30	14.789	2112	2117	2123	rBV2	209773	402765	20.53%	2.070%
31	14.936	2138	2142	2148	rVB	303988	373242	19.02%	1.919%
32	15.301	2198	2204	2211	rVB2	418001	614089	31.30%	3.157%
33	15.707	2268	2273	2276	rBV	331332	429685	21.90%	2.209%
34	15.748	2276	2280	2294	rVB	469973	777504	39.63%	3.997%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

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-BF083018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.177	2348	2353	2360	rVB	221531	346975	17.69%	1.784%
36	16.724	2441	2446	2459	rVB2	104091	211235	10.77%	1.086%

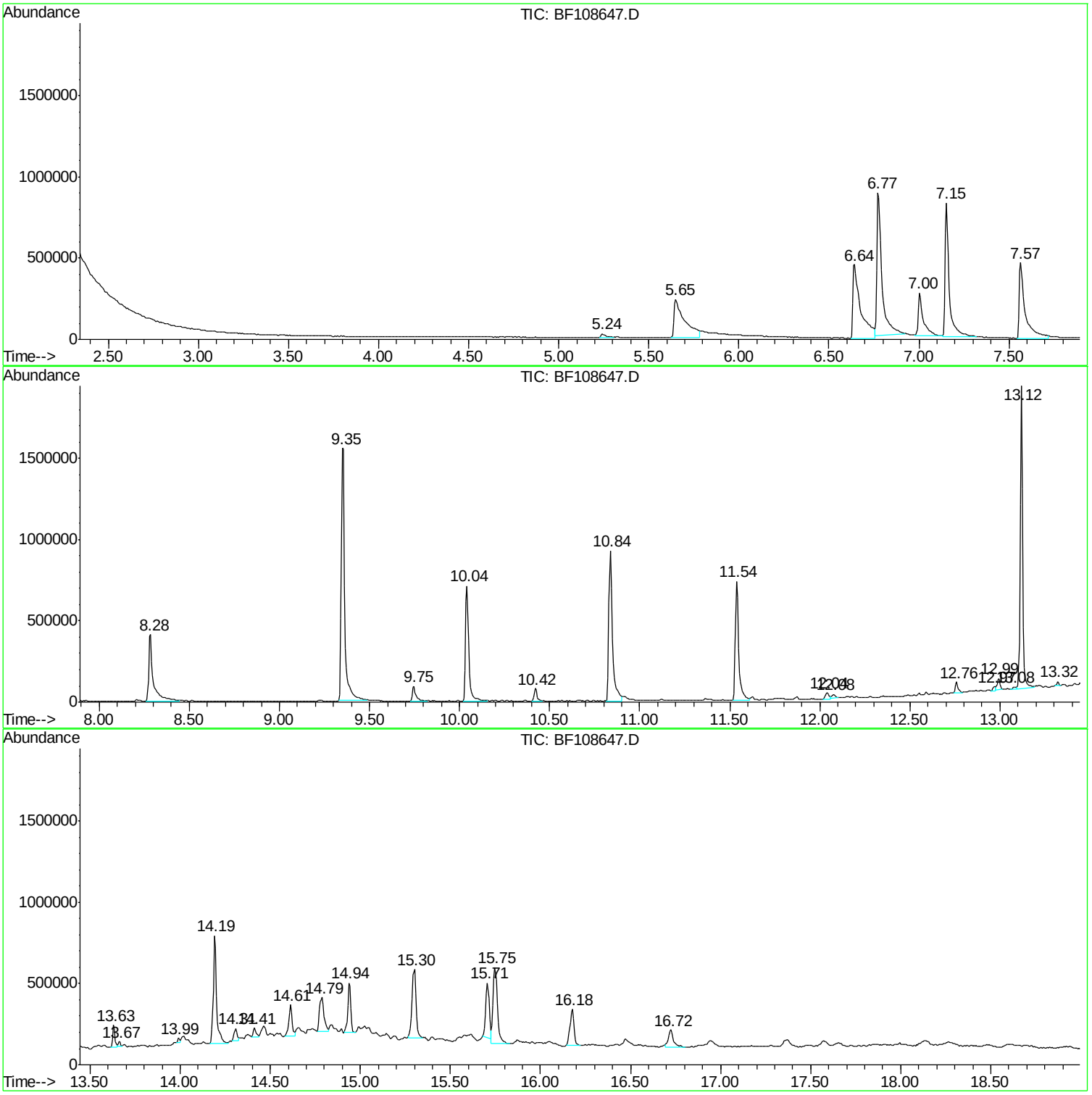
Sum of corrected areas: 19452770

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

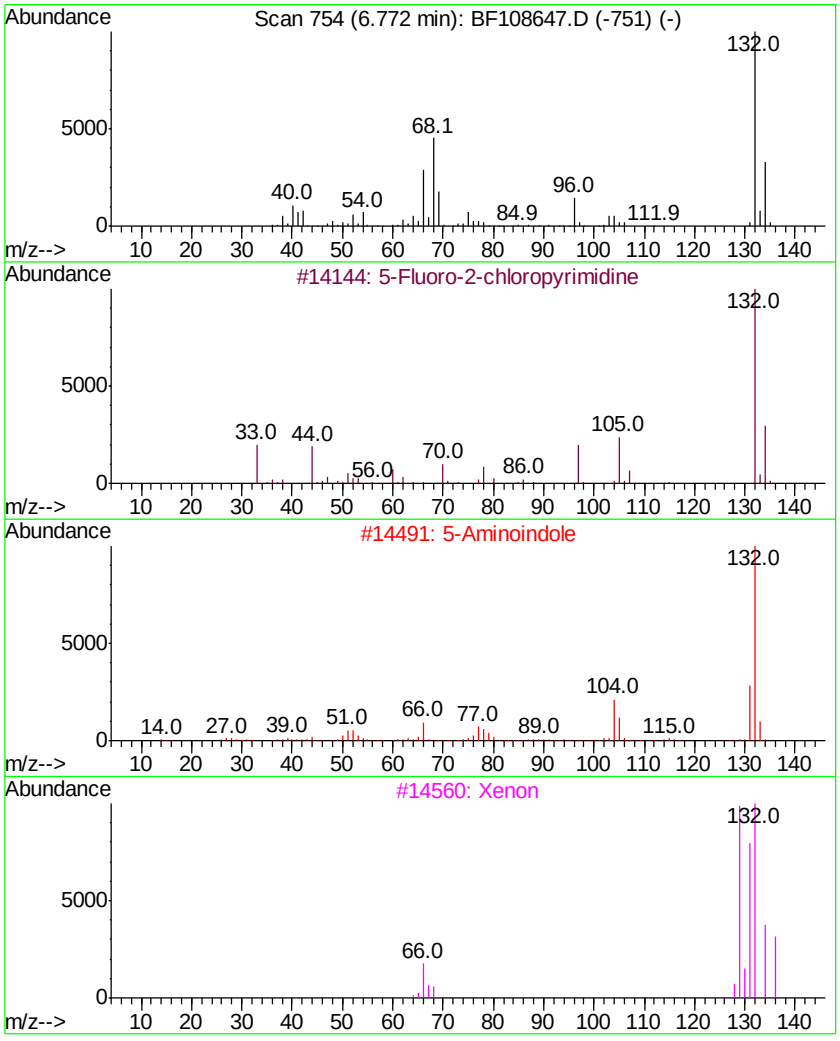
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

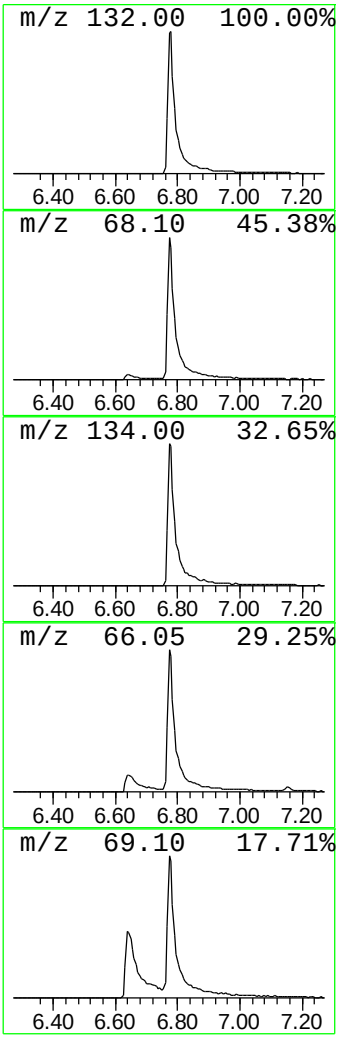
****

Peak Number 1 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	61.63 ng	1651490	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	10
3	Xenon	132	Xe	007440-63-3	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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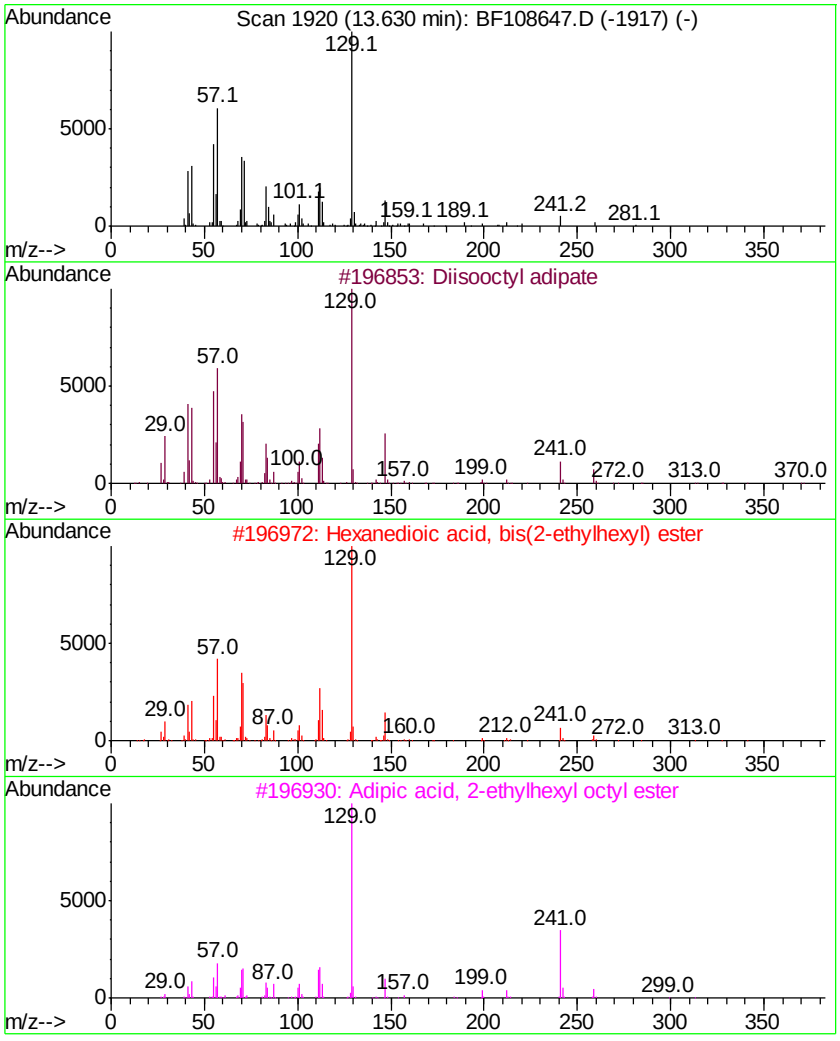
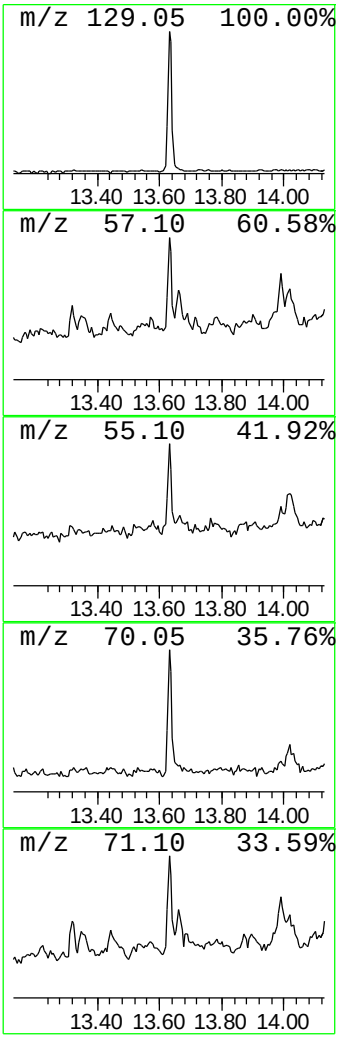
Peak Number 3 Diisooctyl adipate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.84 ng	122146	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisooctyl adipate	370	C22H42O4	001330-86-5	91
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
3	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	64
4	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	62
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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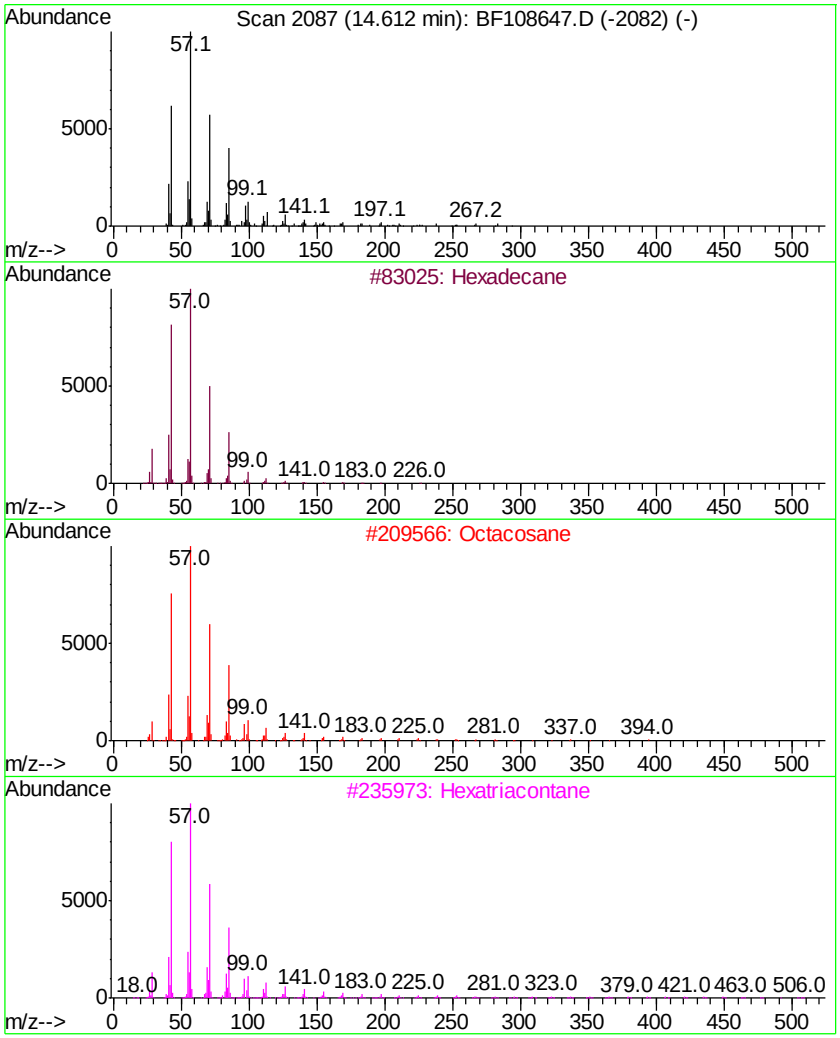
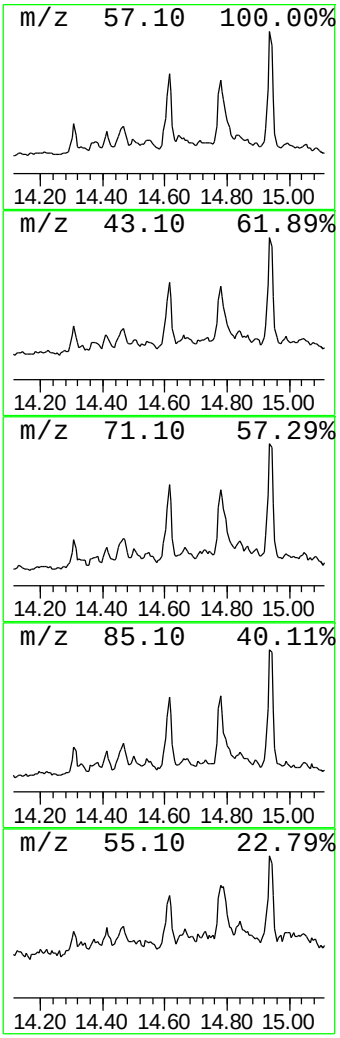
Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	6.03 ng	259188	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexatriacontane	507	C36H74	000630-06-8	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

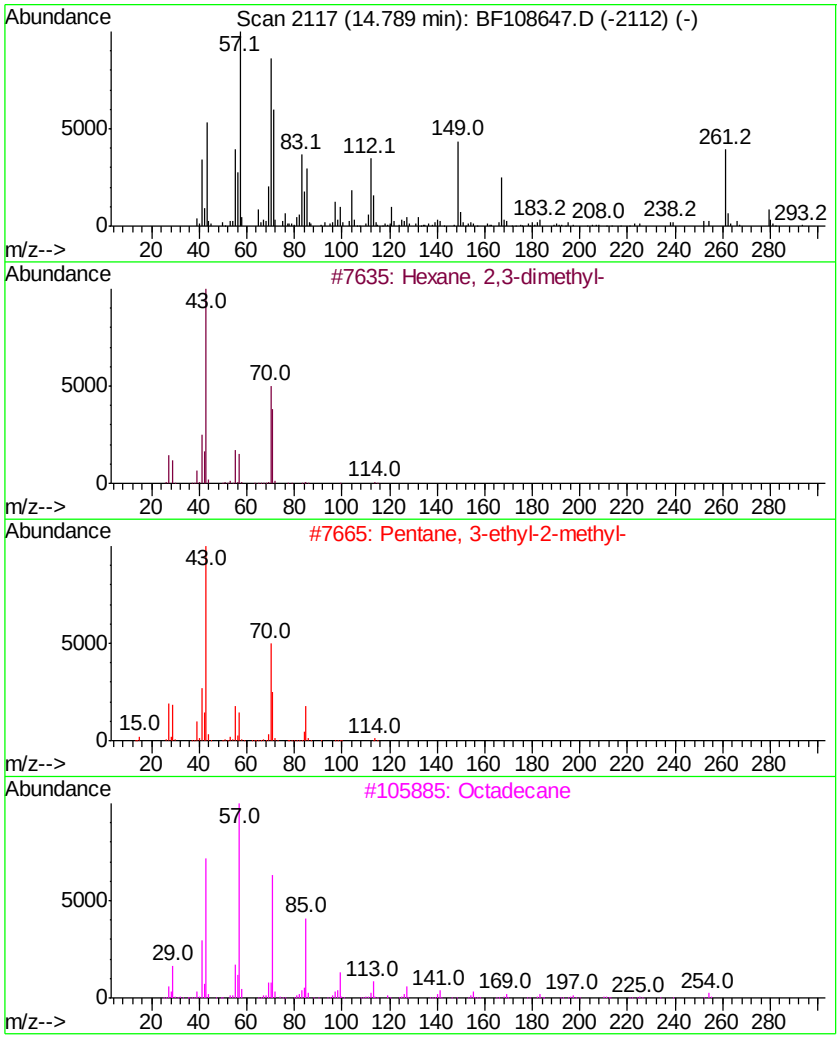
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

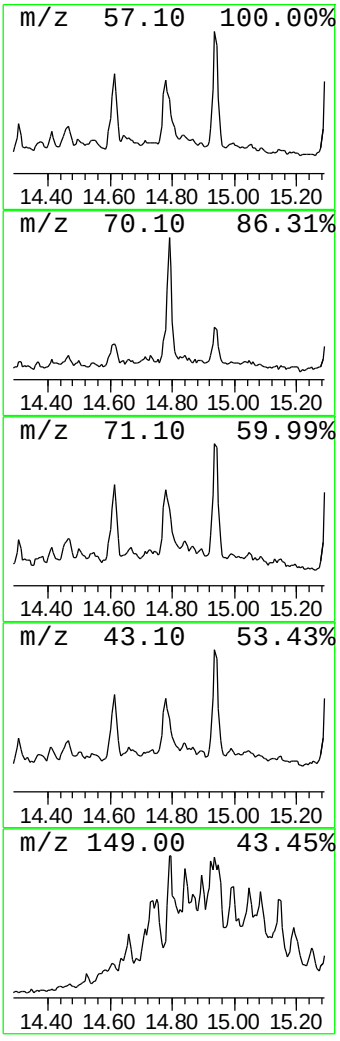
****

Peak Number 5 unknown14.79 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	9.37 ng	402765	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	27
2	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	27
3	Octadecane	254	C18H38	000593-45-3	15
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	11
5	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	11





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

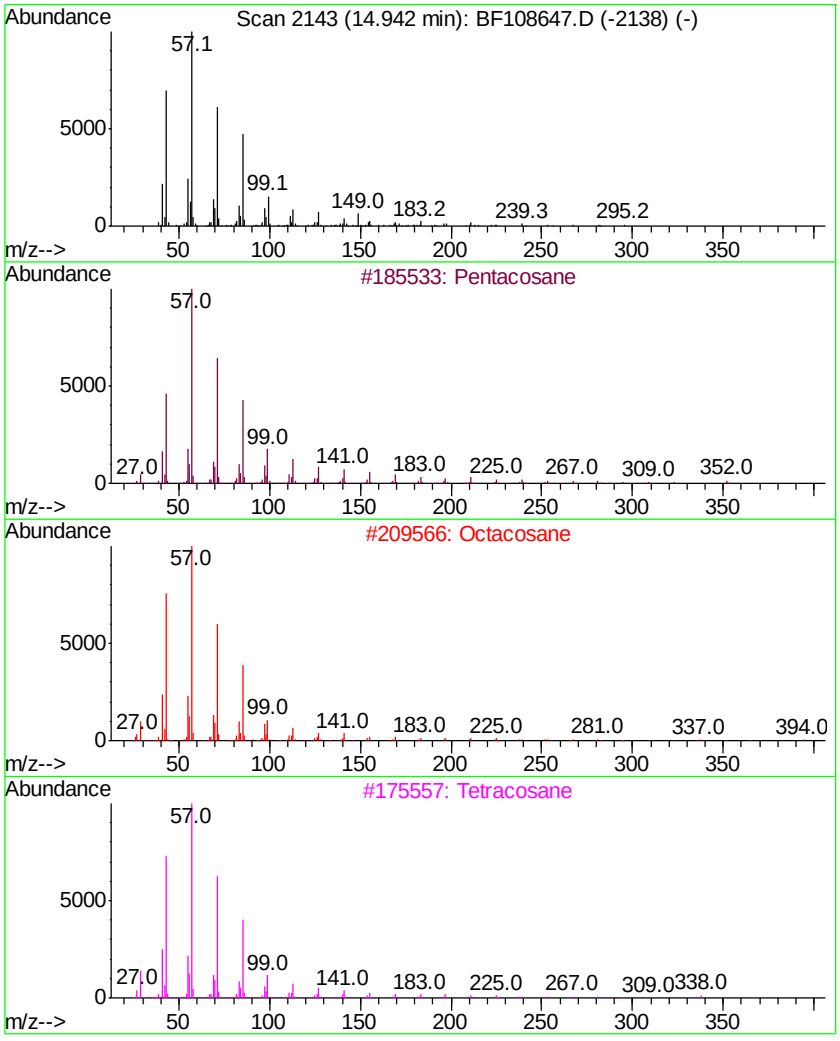
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

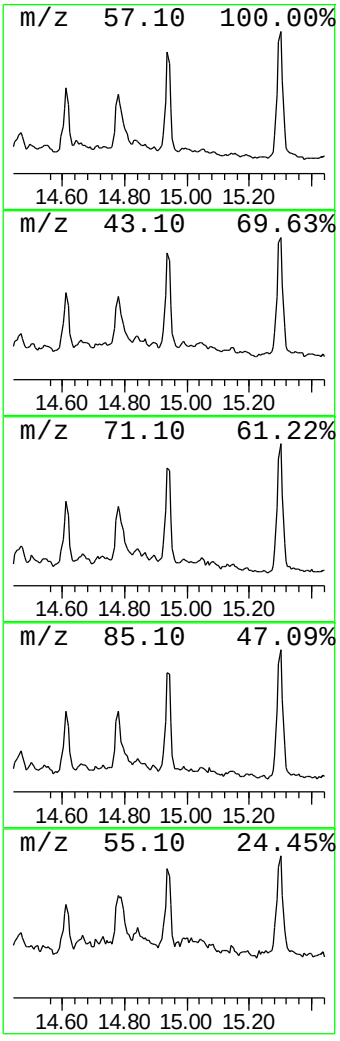
****

Peak Number 6 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	8.68 ng	373242	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Octacosane	394	C28H58	000630-02-4	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Nonadecane	268	C19H40	000629-92-5	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

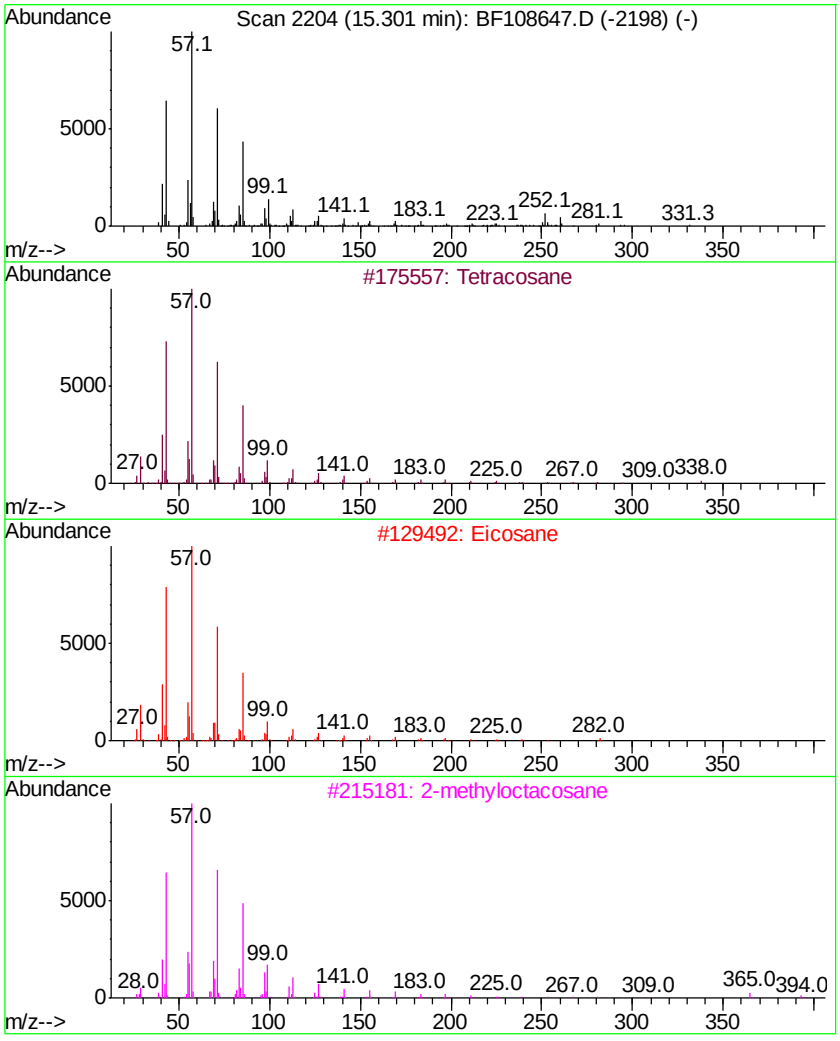
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

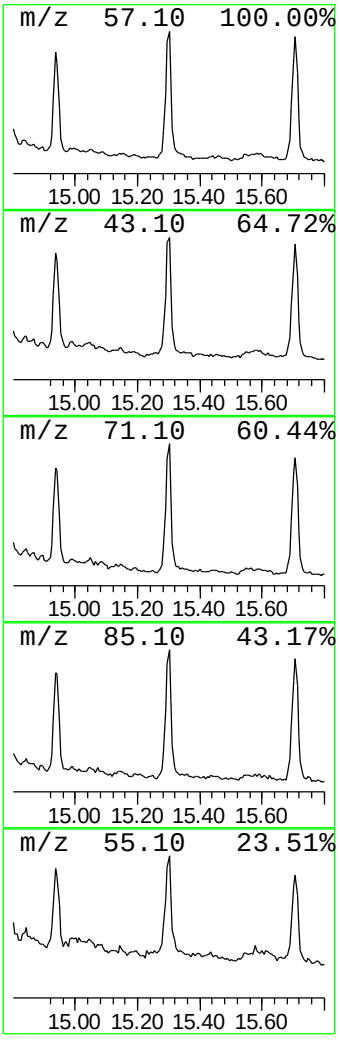
****

Peak Number 7 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	15.80 ng	614089	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Eicosane	282	C20H42	000112-95-8	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

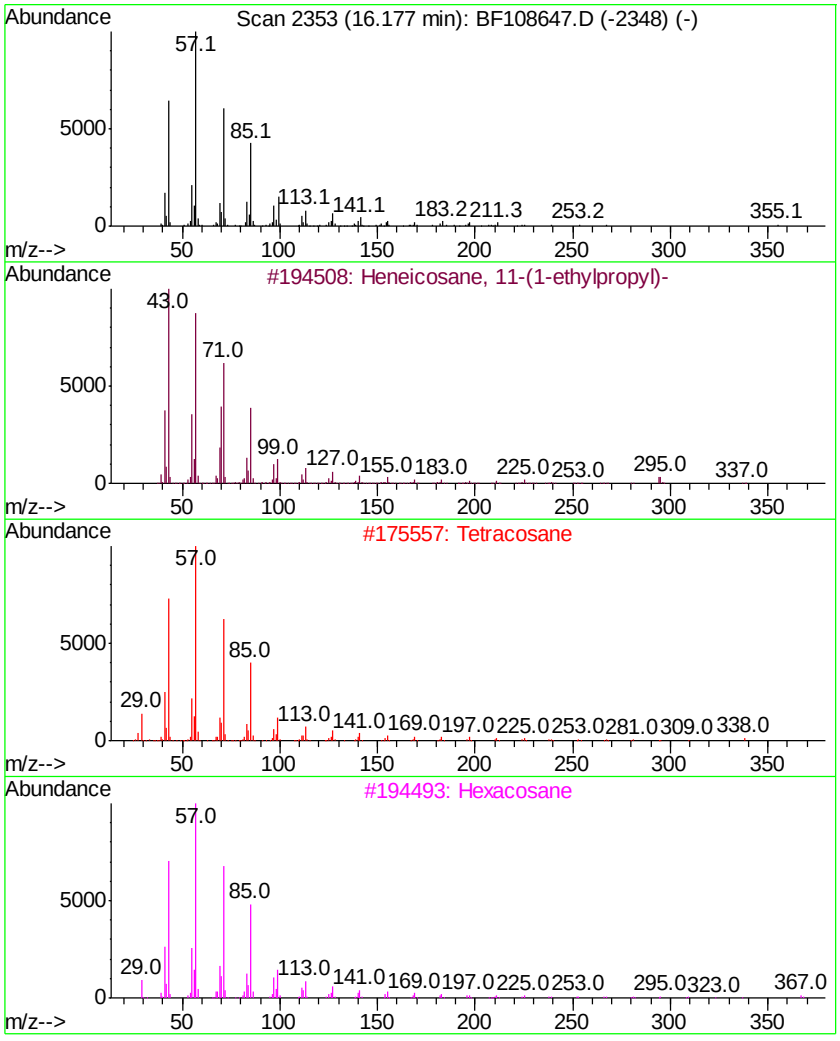
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

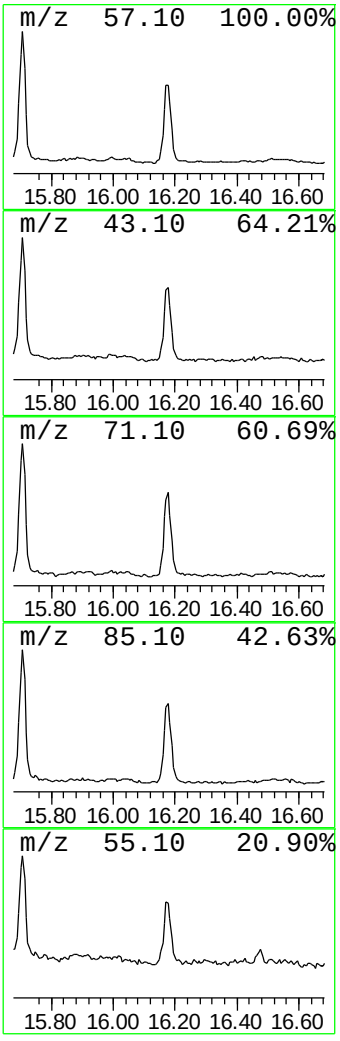
****

Peak Number 8 Heneicosane, 11-(1-ethylpro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	8.93 ng	346975	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octadecane	254	C18H38	000593-45-3	87
5	Eicosane	282	C20H42	000112-95-8	87





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Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

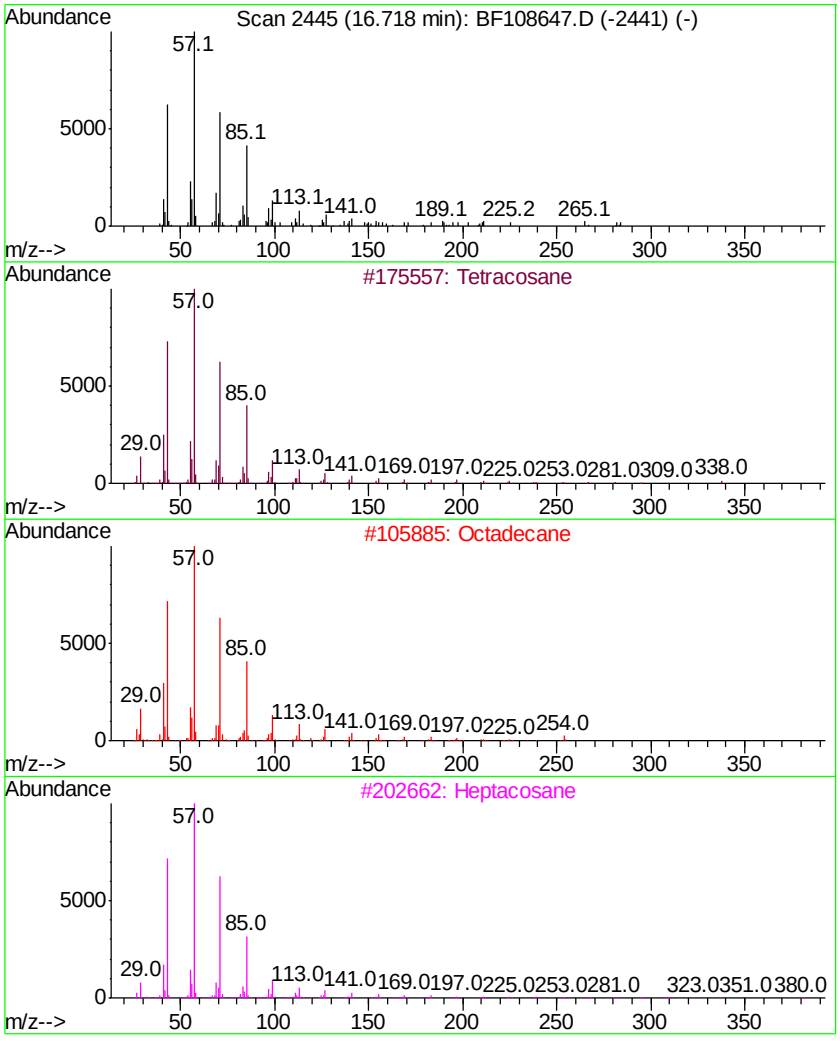
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

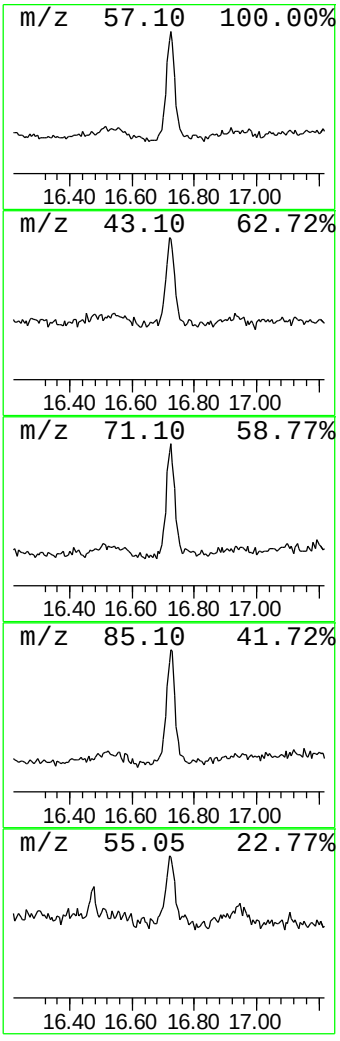
****

Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	5.43 ng	211235	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083018\
Data File : BF108647.D
Acq On : 30 Aug 2018 18:28
Operator : JU/SJ
Sample : J4663-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 6722AA

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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
unknown6.77	6.77	61.6	ng	1651490	1	7.00	535924	20.0
Diisooctyl adipate	13.63	2.8	ng	122146	5	14.19	859825	20.0
Hexadecane	14.61	6.0	ng	259188	5	14.19	859825	20.0
unknown14.79	14.79	9.4	ng	402765	5	14.19	859825	20.0
Pentacosane	14.94	8.7	ng	373242	5	14.19	859825	20.0
Eicosane	15.30	15.8	ng	614089	6	15.75	777504	20.0
Heneicosane, 11-(...	16.18	8.9	ng	346975	6	15.75	777504	20.0
Tetracosane	16.72	5.4	ng	211235	6	15.75	777504	20.0