LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
Operator : JU/SJ
Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7

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-BF110818.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	2.257	23	29	43	rVB	385862	499884	18.62%	2.755%
2	5.175	522	525	532	rBV	34056	44454	1.66%	0.245%
3	5.563	587	591	611	rBV	1006363	977156	36.40%	5.385%
4	6.563	758	761	766	rBV	712273	648187	24.15%	3.572%
5	6.604	766	768	780	rVB	115350	129126	4.81%	0.712%
6	6.710	782	786	790	rBV	1784819	1716169	63.93%	9.457%
7	6.945	822	826	832	rBV	485372	456129	16.99%	2.514%
8	7.098	848	852	867	rVB	1608088	1402093	52.23%	7.726%
9	7.510	917	922	925	rBV	1298896	1253171	46.68%	6.906%
10	7.963	997	999	1003	rVB	39643	35582	1.33%	0.196%
11	8.227	1039	1044	1053	rBV	599526	630713	23.50%	3.476%
12	8.304	1053	1057	1071	rVB	69623	96297	3.59%	0.531%
13	9.298	1221	1226	1229	rBV	2572044	2319503	86.41%	12.782%
14	9.692	1289	1293	1299	rBV	36261	32910	1.23%	0.181%
15	9.986	1338	1343	1352	rVB	733422	727945	27.12%	4.011%
16	10.780	1473	1478	1490	rBV	1612369	1557470	58.02%	8.583%
17	11.480	1593	1597	1604	rBV	839504	780078	29.06%	4.299%
18	11.980	1679	1682	1686	rBV	72785	70049	2.61%	0.386%
19	12.215	1718	1722	1728	rVB2	51722	53128	1.98%	0.293%
20	12.321	1737	1740	1746	rVB	179154	170564	6.35%	0.940%
21	12.721	1806	1808	1811	rVB	46036	35005	1.30%	0.193%
22	12.768	1813	1816	1822	rBV3	34335	43498	1.62%	0.240%
23	13.062	1861	1866	1869	rBV	2677568	2684314	100.00%	14.792%
24	13.933	2011	2014	2021	rBV	133774	150963	5.62%	0.832%
25	14.127	2043	2047	2056	rBV	636143	619531	23.08%	3.414%
26	14.257	2065	2069	2072	rVB	26414	27109	1.01%	0.149%
27	14.557	2117	2120	2127	rBV	49182	58122	2.17%	0.320%
28	14.874	2171	2174	2179	rVB	77453	74784	2.79%	0.412%
29	15.227	2229	2234	2238	rBV	90025	111261	4.14%	0.613%
30	15.621	2296	2301	2303	rBV	98091	125257	4.67%	0.690%
31	15.656	2303	2307	2317	rVB	269398	383847	14.30%	2.115%
32	16.074	2371	2378	2384	rBV	81936	129448	4.82%	0.713%
33	16.603	2462	2468	2473	rBV	40119	75176	2.80%	0.414%
34	17.227	2568	2574	2579	rBV3	13809	27983	1.04%	0.154%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
Operator : JU/SJ
Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

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-BF110818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

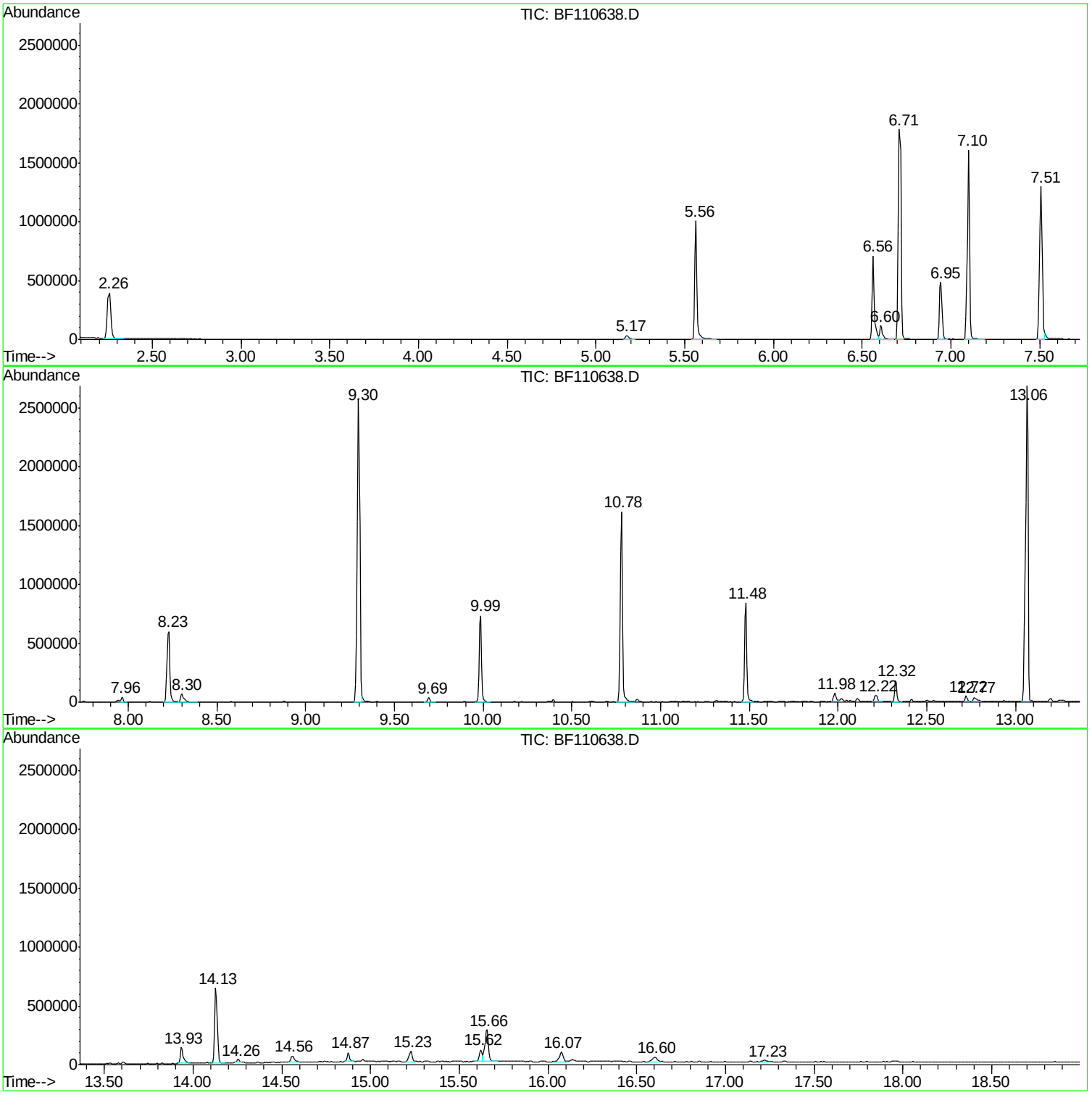
Sum of corrected areas: 18146906

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
Operator : JU/SJ
Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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\BF110918\
Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
Operator : JU/SJ
Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

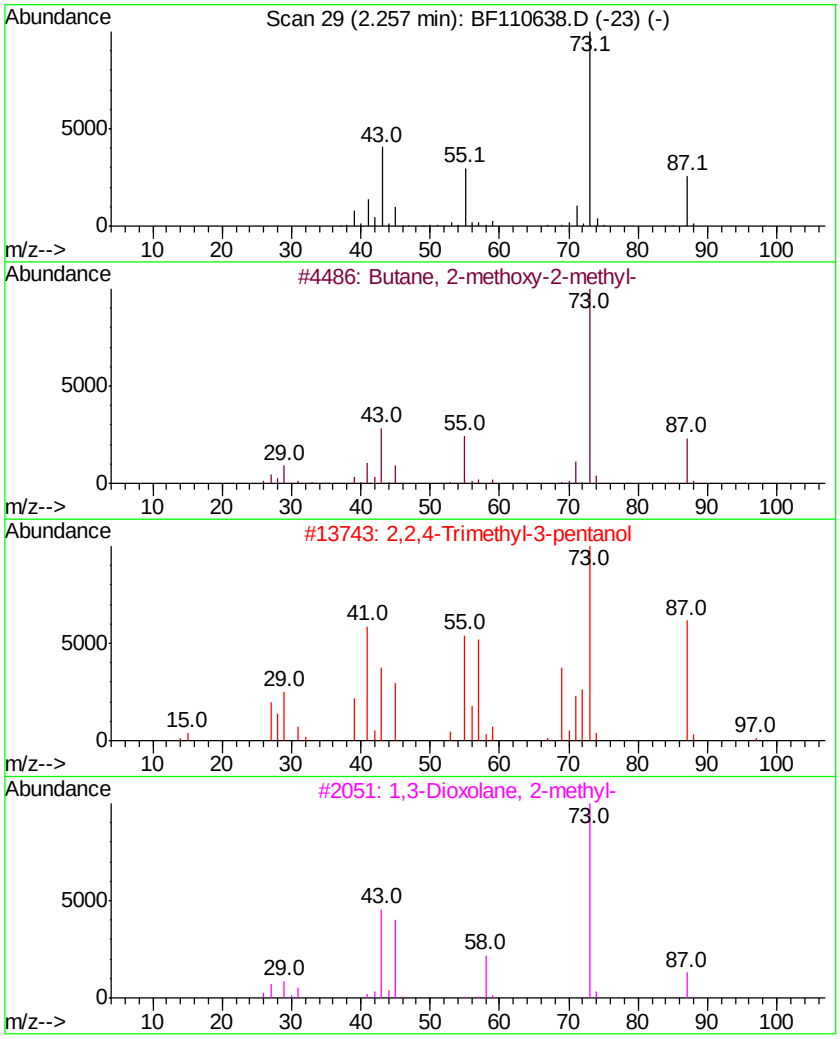
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

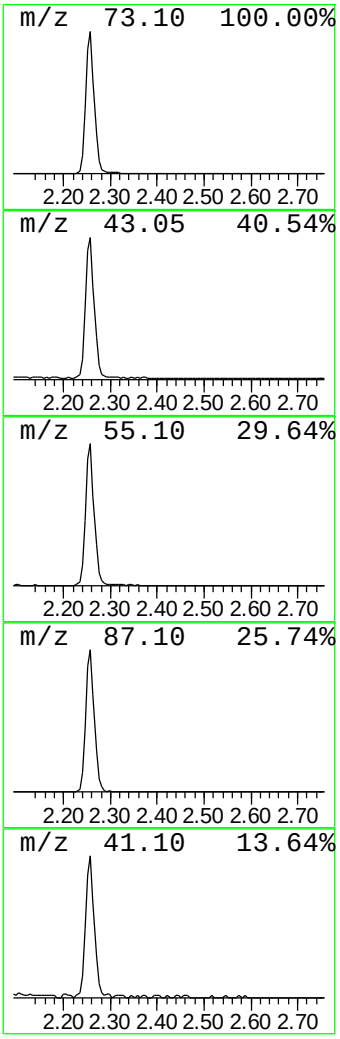
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	21.92 ng	499884	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
Operator : JU/SJ
Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

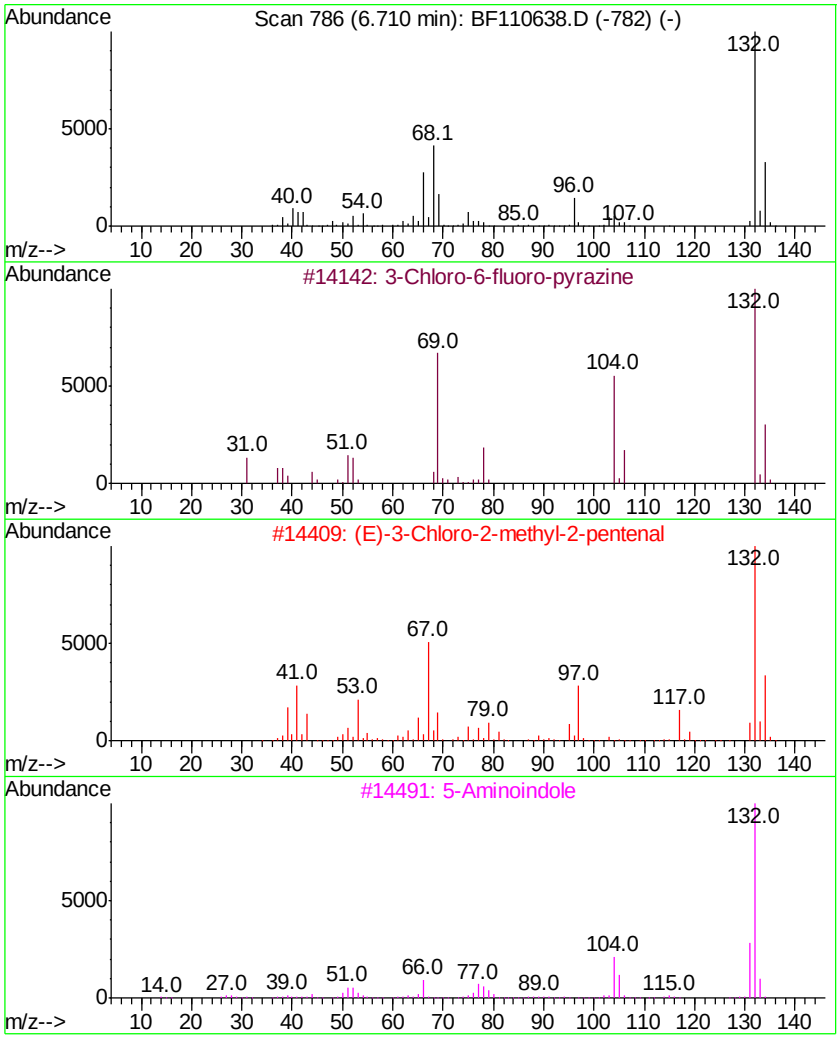
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

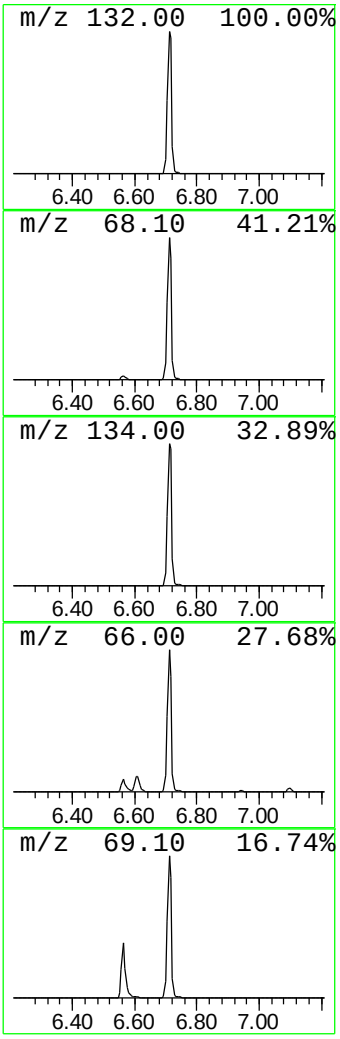
****

Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	75.25 ng	1716170	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
Operator : JU/SJ
Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

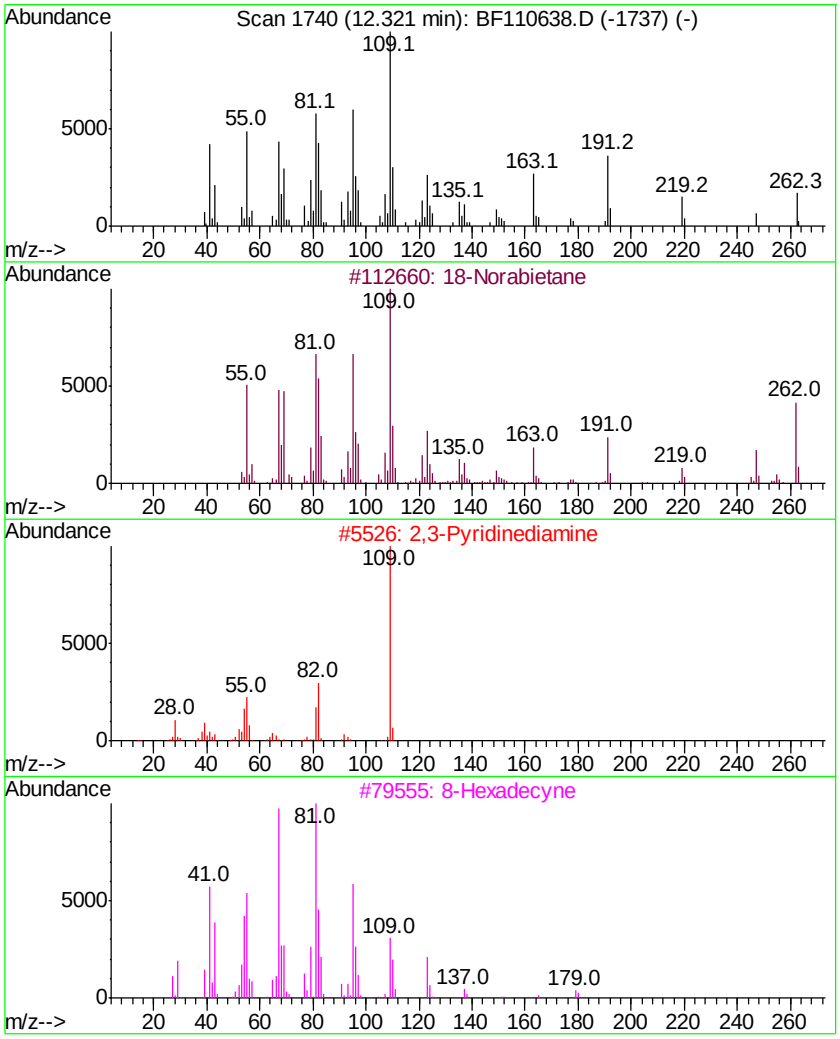
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

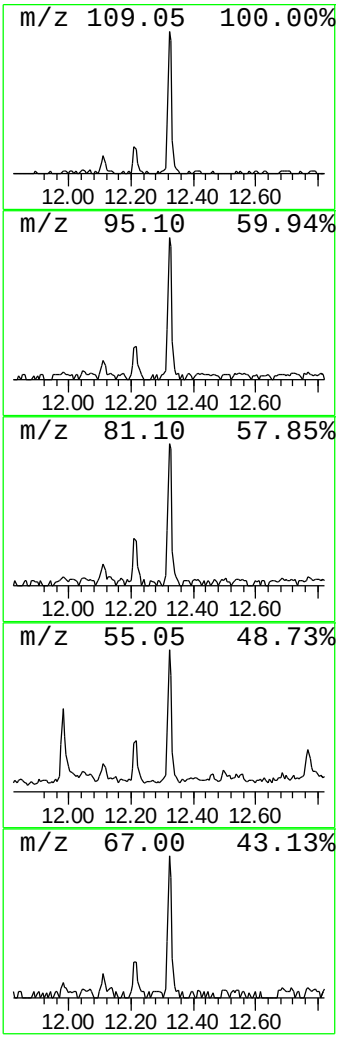
****

Peak Number 4 18-Norabietane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	4.37 ng	170564	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	18-Norabietane	262	C19H34	1000293-16-6	96
2	2,3-Pyridinediamine	109	C5H7N3	000452-58-4	35
3	8-Hexadecyne	222	C16H30	019781-86-3	35
4	1H-Pyrazole, 4-(2-bromoethyl)-3,...	202	C7H11BrN2	083467-28-1	27
5	2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
Operator : JU/SJ
Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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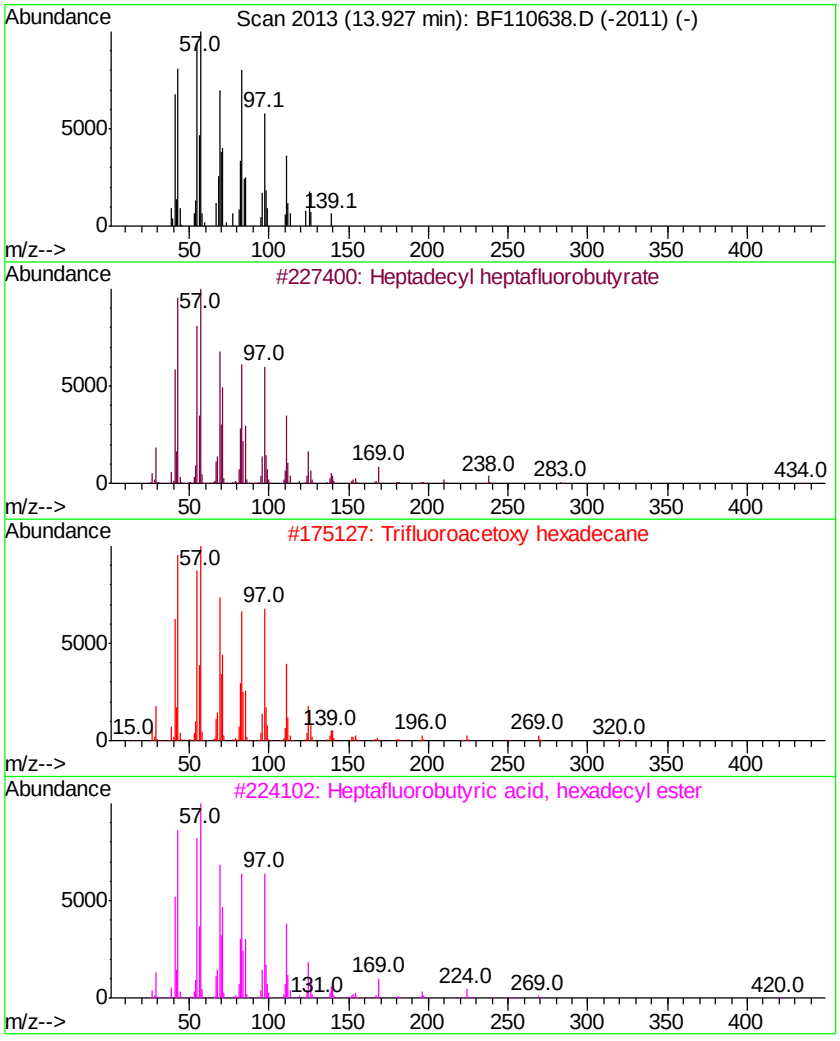
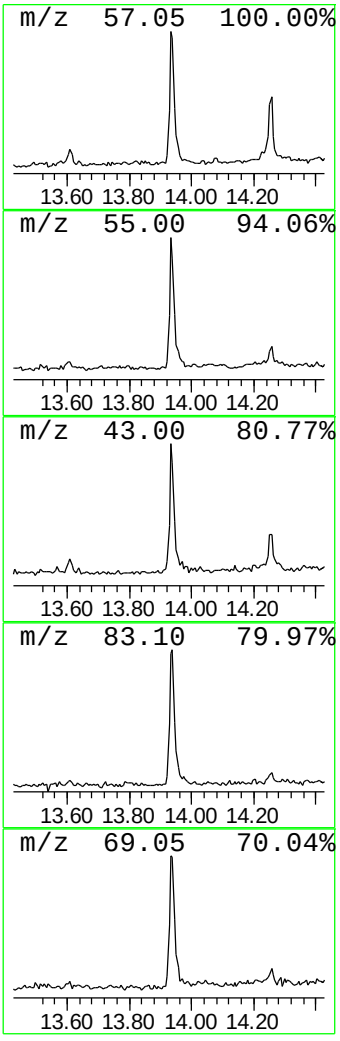
Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	4.87 ng	150963	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

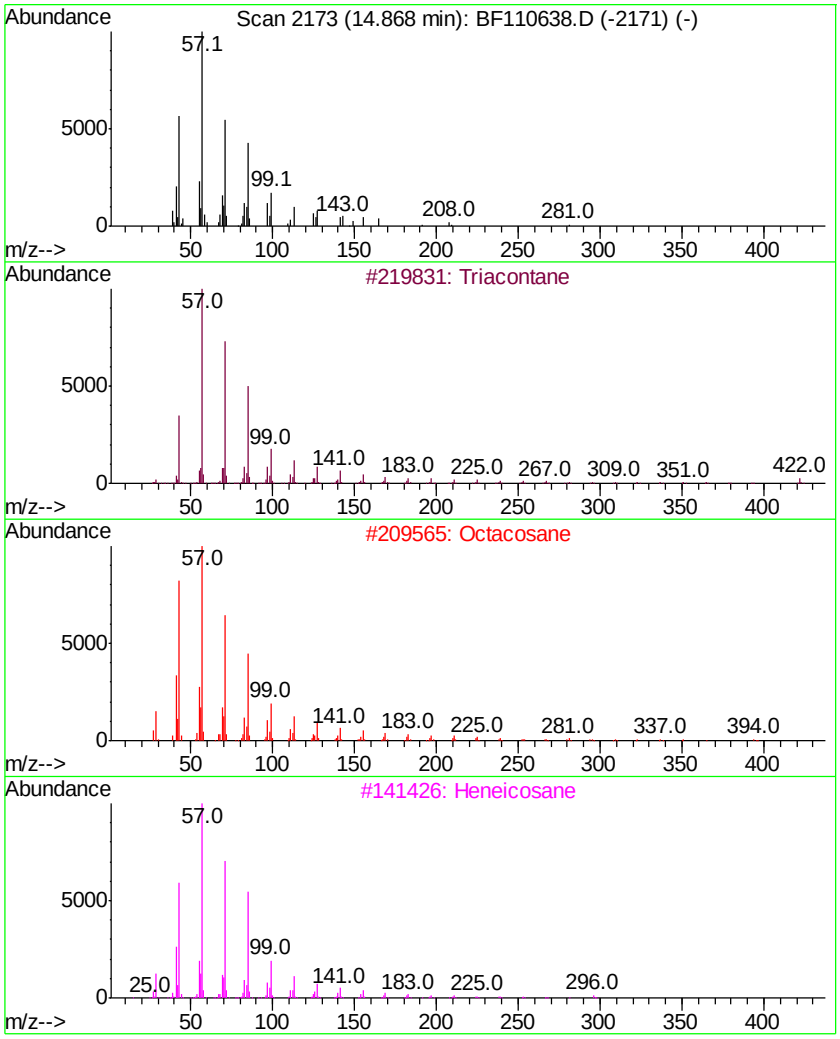
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

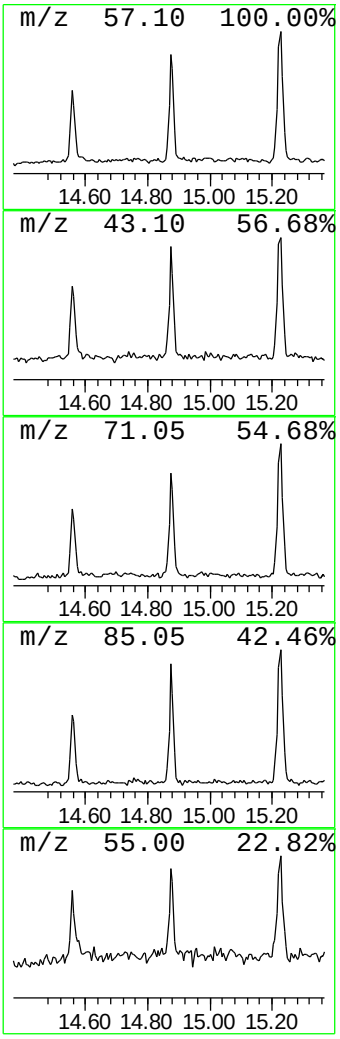
****

Peak Number 6 Triacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.41 ng	74784	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





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Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
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Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

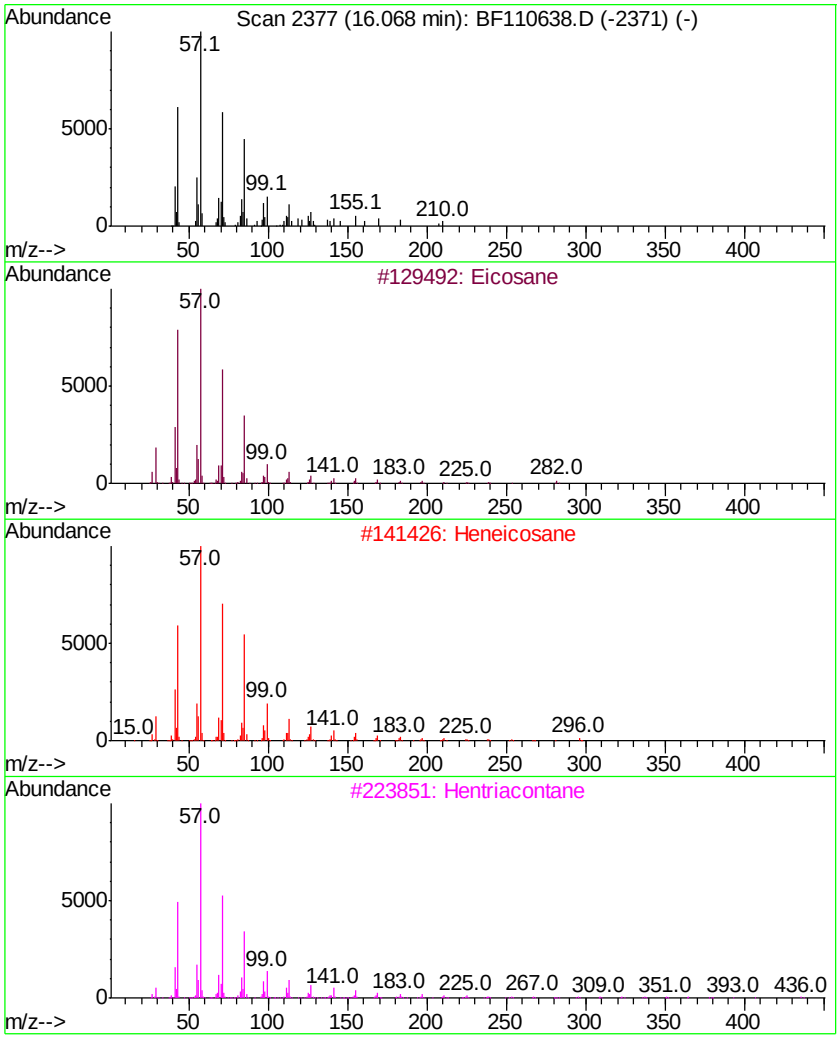
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

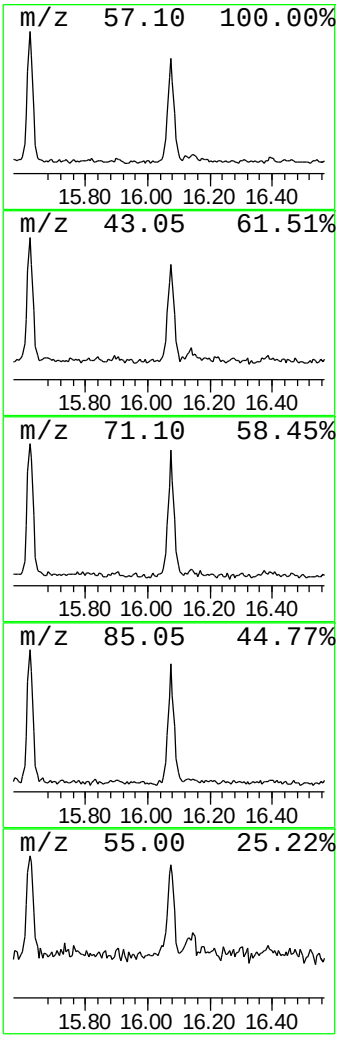
****

Peak Number 8 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	6.74 ng	129448	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Octadecane	254	C18H38	000593-45-3	91





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Operator : JU/SJ
Sample : J5884-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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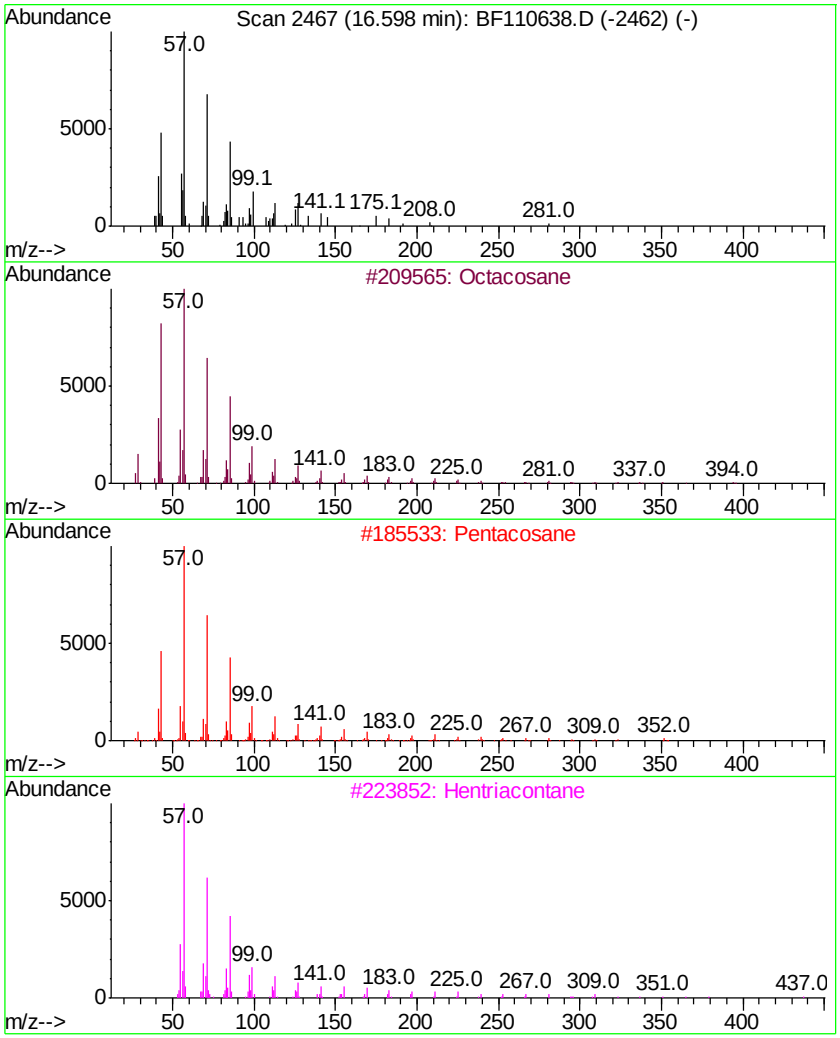
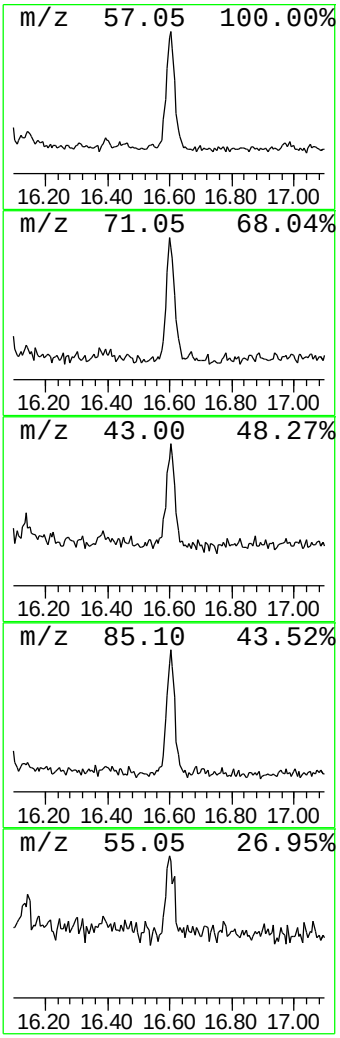
Peak Number 9 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	3.92 ng	75176	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Hexacosane	366	C26H54	000630-01-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
Data File : BF110638.D
Acq On : 9 Nov 2018 20:14
Operator : JU/SJ
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Instrument : BNA_F
ClientSampleId : TP-7

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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
Butane, 2-methoxy...	2.26	21.9	ng	499884	1	6.95	456129	20.0
unknown6.71	6.71	75.3	ng	1716170	1	6.95	456129	20.0
18-Norabietane	12.32	4.4	ng	170564	4	11.48	780078	20.0
Heptadecyl heptaf...	13.93	4.9	ng	150963	5	14.13	619531	20.0
Triacontane	14.87	2.4	ng	74784	5	14.13	619531	20.0
Eicosane	16.07	6.7	ng	129448	6	15.66	383847	20.0
Octacosane	16.60	3.9	ng	75176	6	15.66	383847	20.0