LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109051.D
Acq On : 17 Sep 2018 16:34
Operator : JU/SJ
Sample : J4929-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-PIT-12

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-BF091418.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	4.919	436	439	446	rBV	97750	129091	3.89%	0.449%
2	5.337	504	510	513	rBV	2909713	3079095	92.71%	10.713%
3	6.360	678	684	688	rBV	3181742	3240046	97.56%	11.273%
4	6.489	702	706	709	rBV	3325791	3179880	95.74%	11.064%
5	6.719	742	745	749	rBV	1020484	893761	26.91%	3.110%
6	6.878	768	772	776	rBV	2819904	2519934	75.87%	8.767%
7	7.283	836	841	844	rBV	2218024	2009916	60.52%	6.993%
8	8.001	959	963	967	rBV	1313001	1070675	32.24%	3.725%
9	9.077	1142	1146	1150	rBV	3606541	3321204	100.00%	11.555%
10	9.472	1210	1213	1216	rBV	299125	242608	7.30%	0.844%
11	9.754	1257	1261	1264	rBV	1215358	1084792	32.66%	3.774%
12	10.536	1390	1394	1397	rBV	1978890	1729758	52.08%	6.018%
13	11.224	1508	1511	1515	rBV	1051285	980220	29.51%	3.410%
14	11.766	1600	1603	1607	rBV	43763	40762	1.23%	0.142%
15	12.813	1776	1781	1784	rBV	2766005	2519524	75.86%	8.766%
16	13.060	1817	1823	1826	rBV	41171	45180	1.36%	0.157%
17	13.395	1878	1880	1883	rBV	55651	50584	1.52%	0.176%
18	13.724	1932	1936	1946	rBV	143423	198840	5.99%	0.692%
19	13.854	1954	1958	1961	rBV	1072137	942557	28.38%	3.279%
20	14.042	1986	1990	1993	rBV	88648	83237	2.51%	0.290%
21	14.342	2038	2041	2044	rBV	96205	85577	2.58%	0.298%
22	14.636	2088	2091	2100	rVB	91665	98634	2.97%	0.343%
23	14.707	2100	2103	2107	rVB	160696	152142	4.58%	0.529%
24	14.954	2142	2145	2150	rVB	76201	94802	2.85%	0.330%
25	15.254	2192	2196	2202	rVV	653638	798556	24.04%	2.778%
26	15.312	2202	2206	2211	rVB	73864	91837	2.77%	0.320%
27	15.718	2272	2275	2279	rVB	46935	58639	1.77%	0.204%

Sum of corrected areas: 28741851

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
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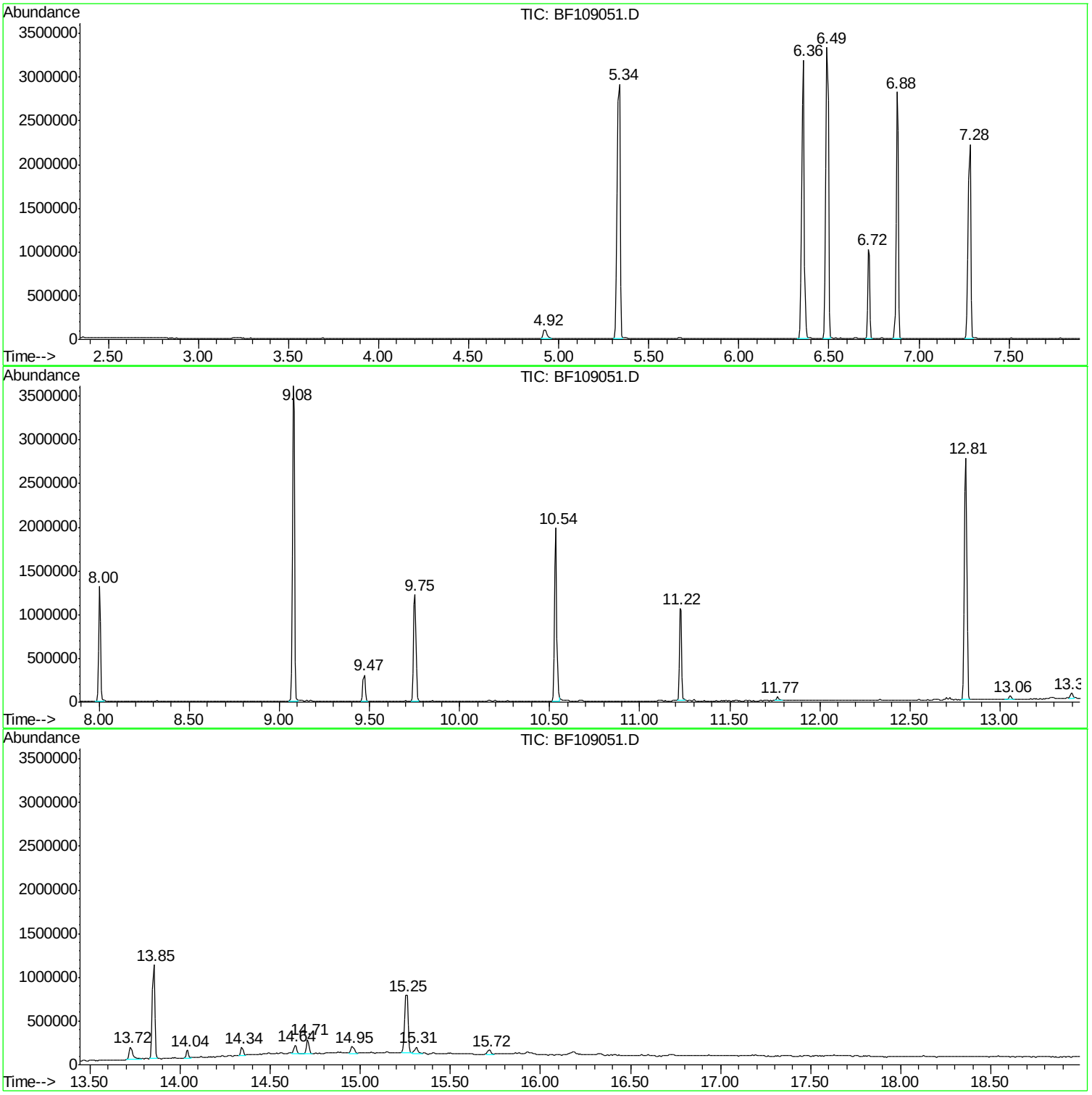
Acq On : 17 Sep 2018 16:34
Operator : JU/SJ
Sample : J4929-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-PIT-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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\BF091718\
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Acq On : 17 Sep 2018 16:34
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-PIT-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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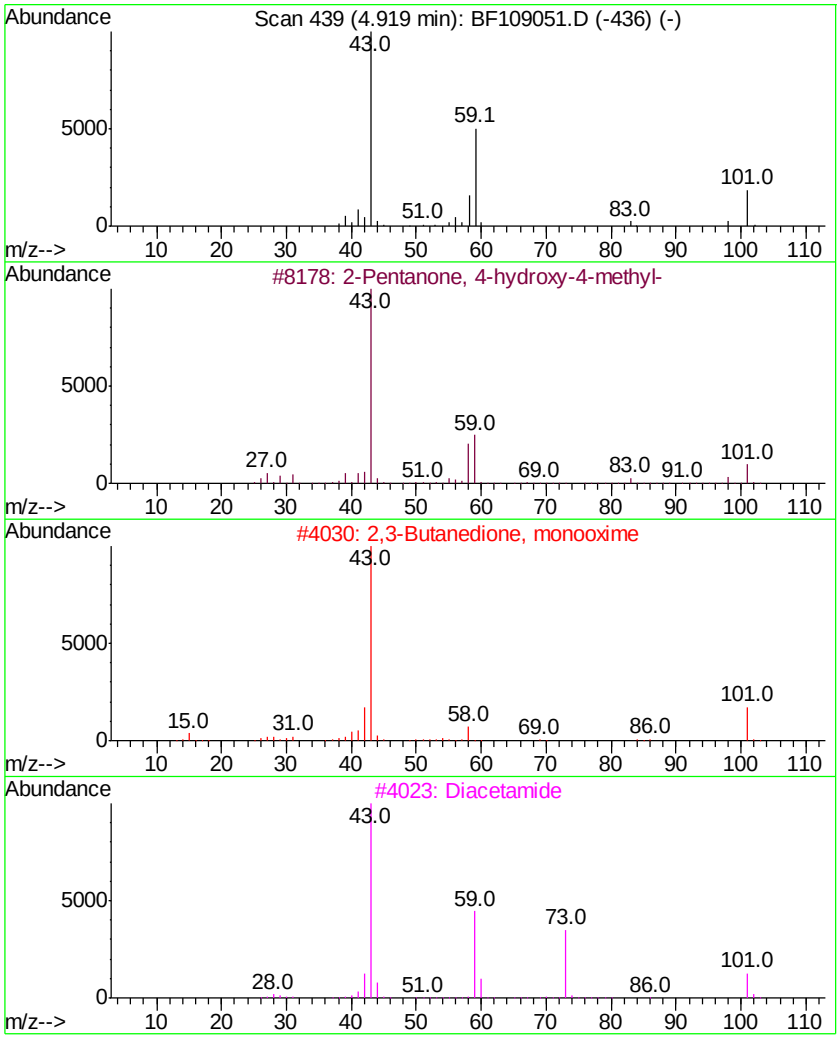
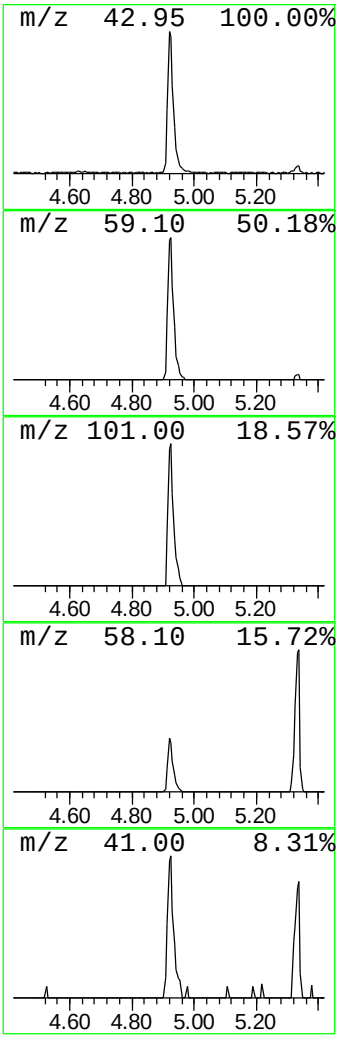
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.89 ng	129091	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
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Operator : JU/SJ
Sample : J4929-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-PIT-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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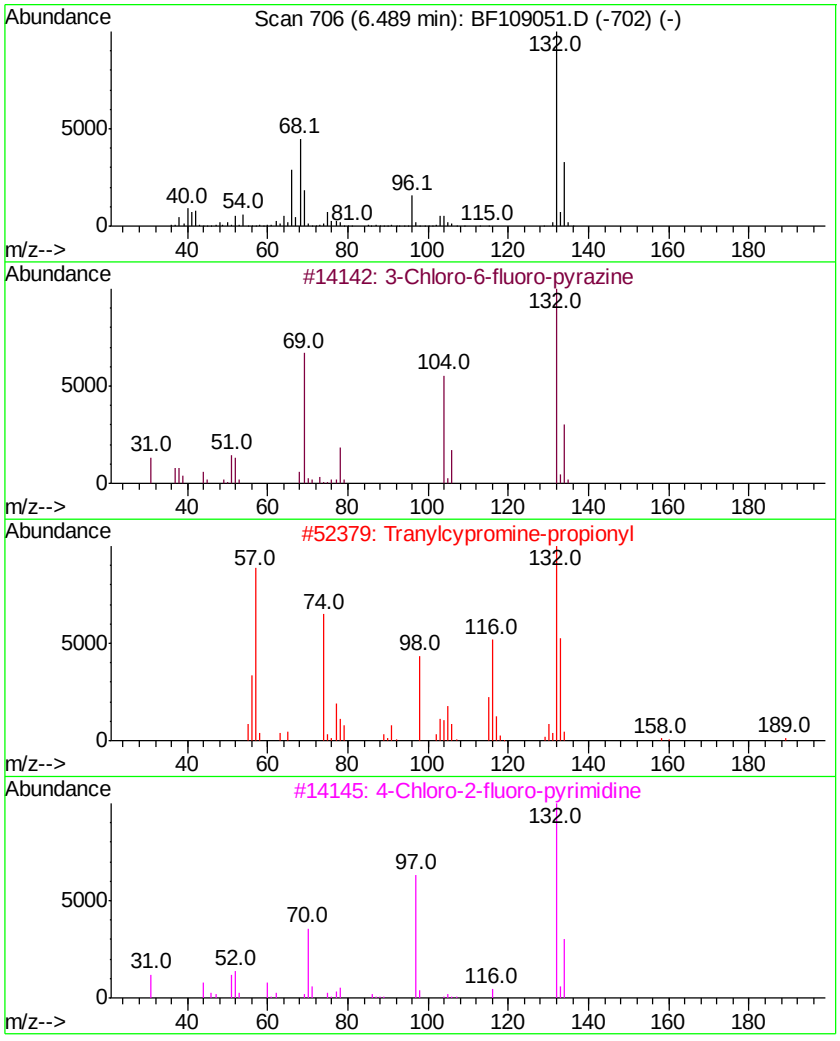
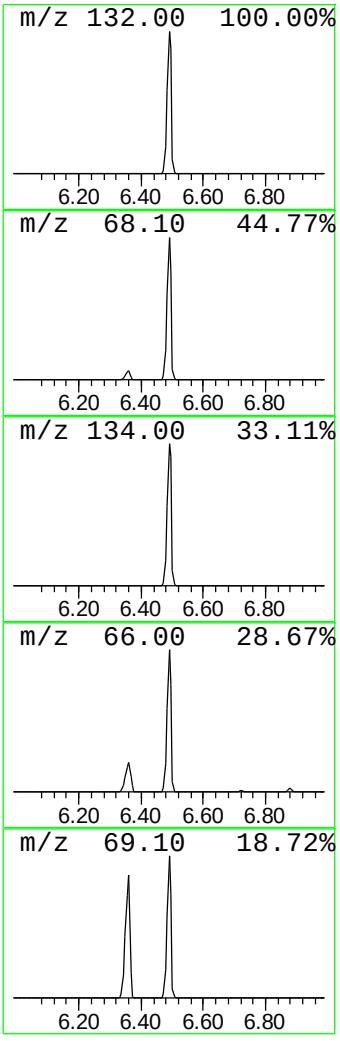
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	71.16 ng	3179880	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Data File : BF109051.D
Acq On : 17 Sep 2018 16:34
Operator : JU/SJ
Sample : J4929-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-PIT-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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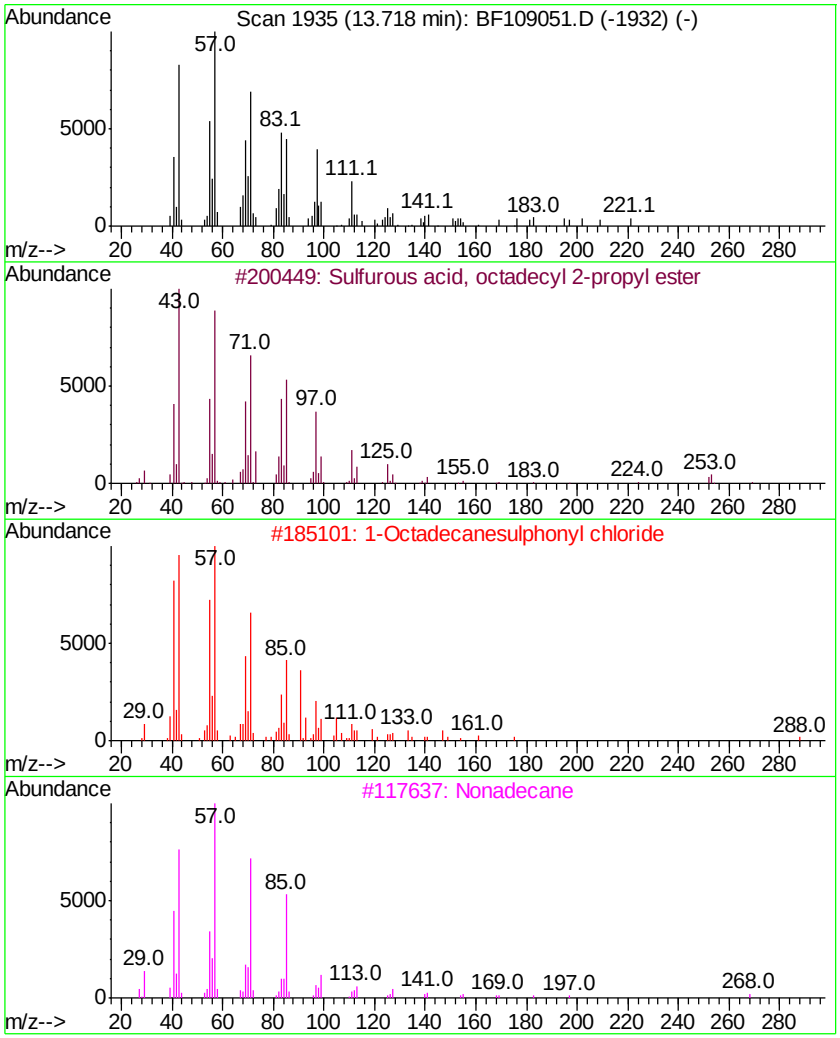
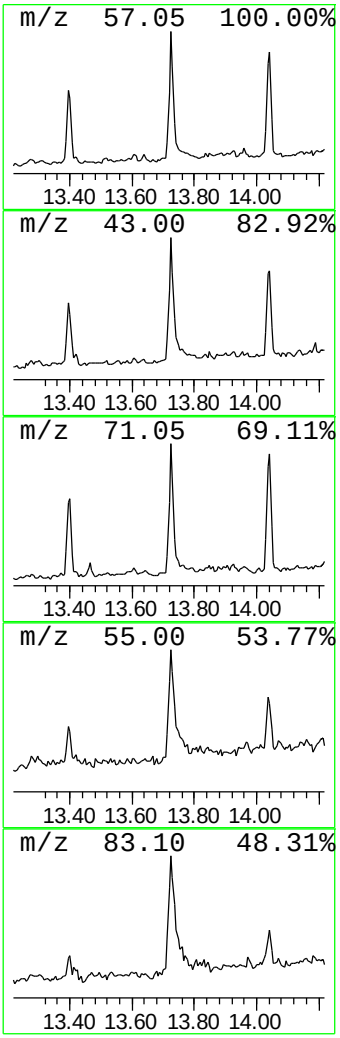
Peak Number 4 Sulfurous acid, octadecyl 2... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.22 ng	198840	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	86
3	Nonadecane	268	C19H40	000629-92-5	72
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	68
5	Hexadecane	226	C16H34	000544-76-3	64





Library Search Compound Report

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Operator : JU/SJ
Sample : J4929-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-PIT-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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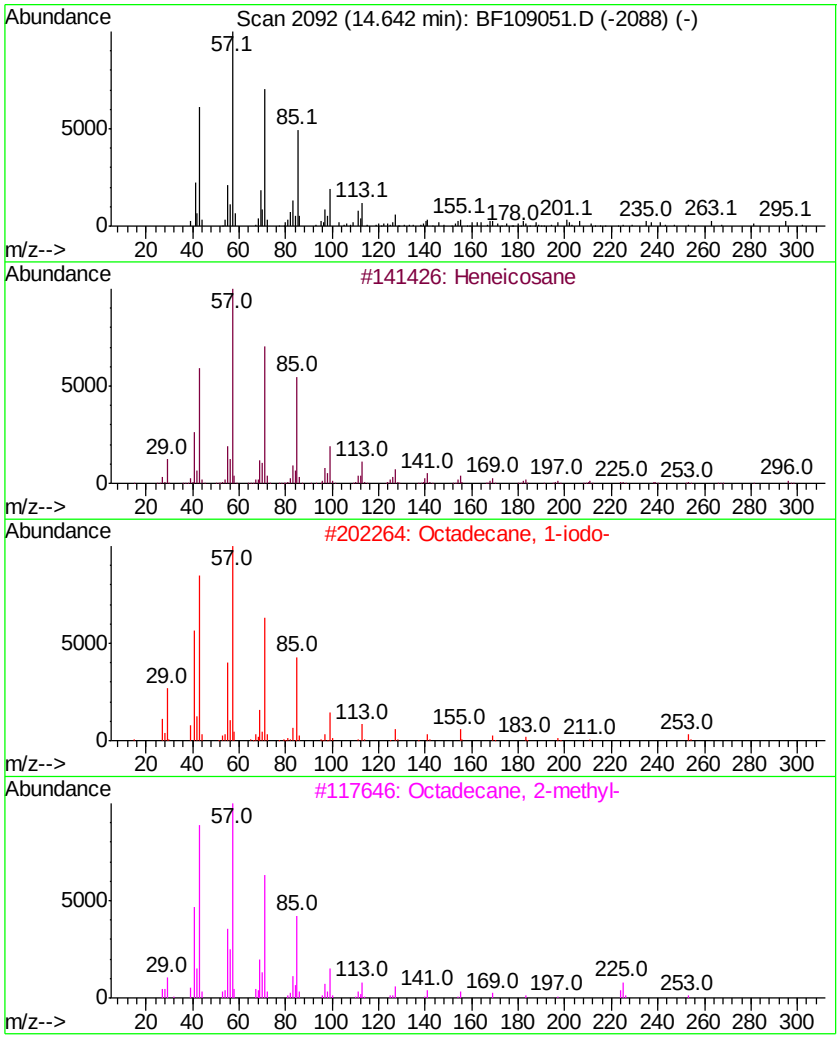
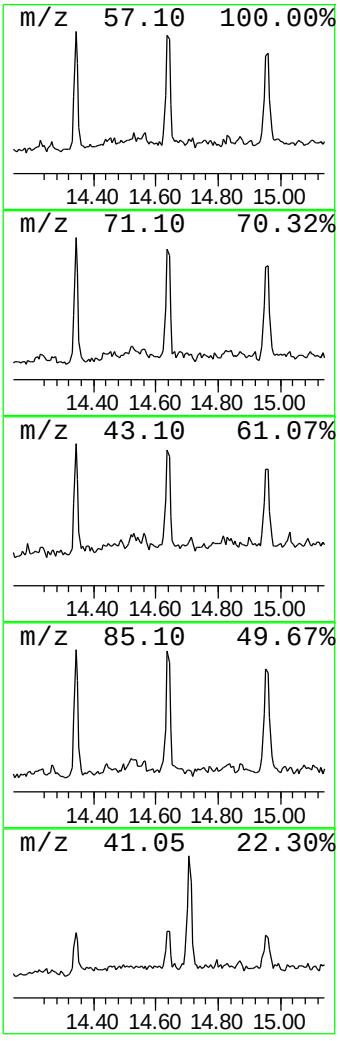
Peak Number 5 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.47 ng	98634	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
5	Tetratetracontane	619	C44H90	007098-22-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091718\
Data File : BF109051.D
Acq On : 17 Sep 2018 16:34
Operator : JU/SJ
Sample : J4929-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-PIT-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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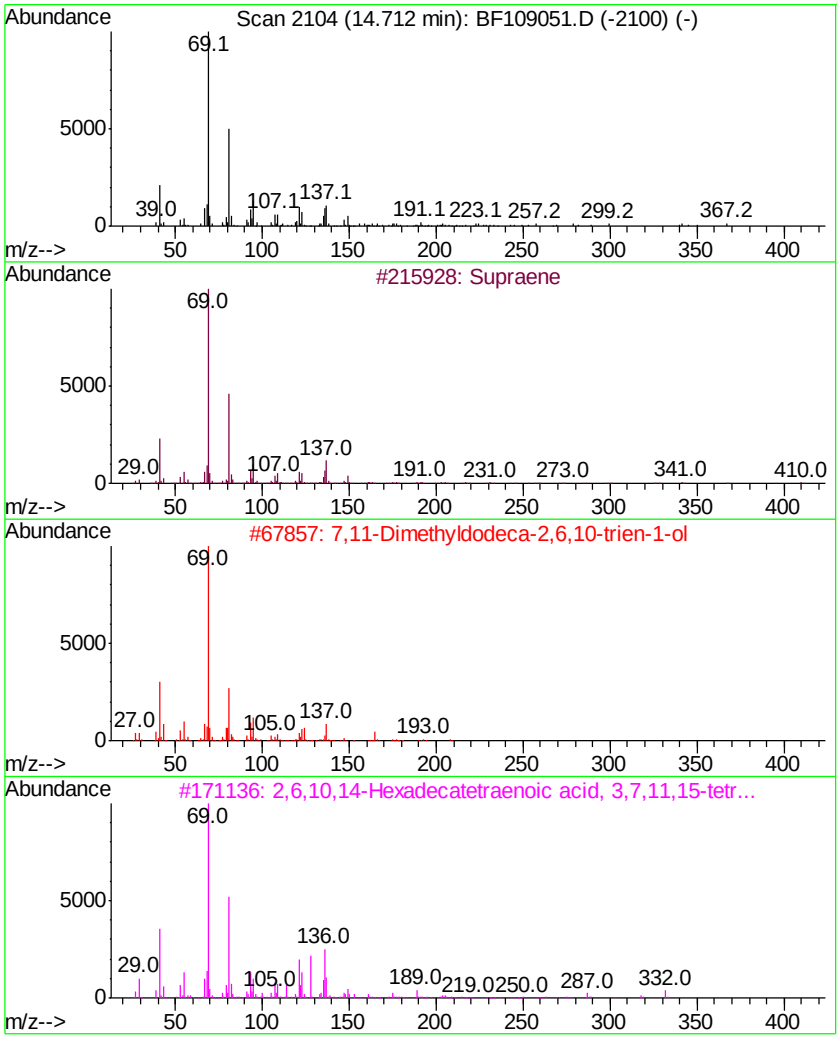
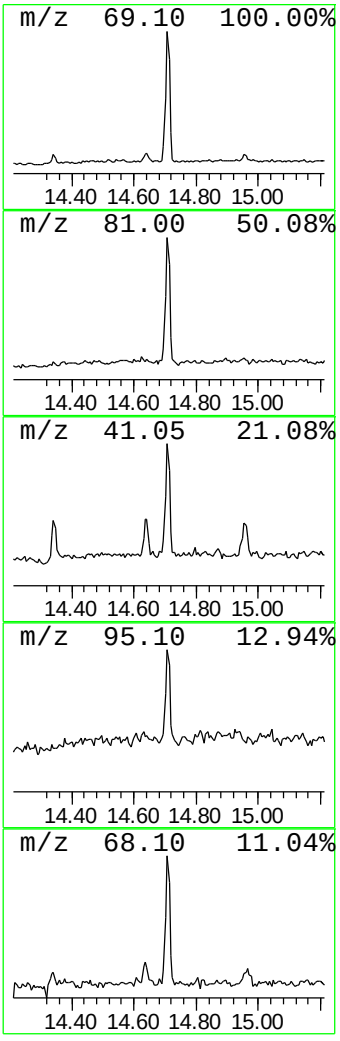
Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.81 ng	152142	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
5	(E)-2-Butenoic acid, 2-(methylen...	180	C11H16O2	1000158-24-3	50





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Sample : J4929-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-PIT-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

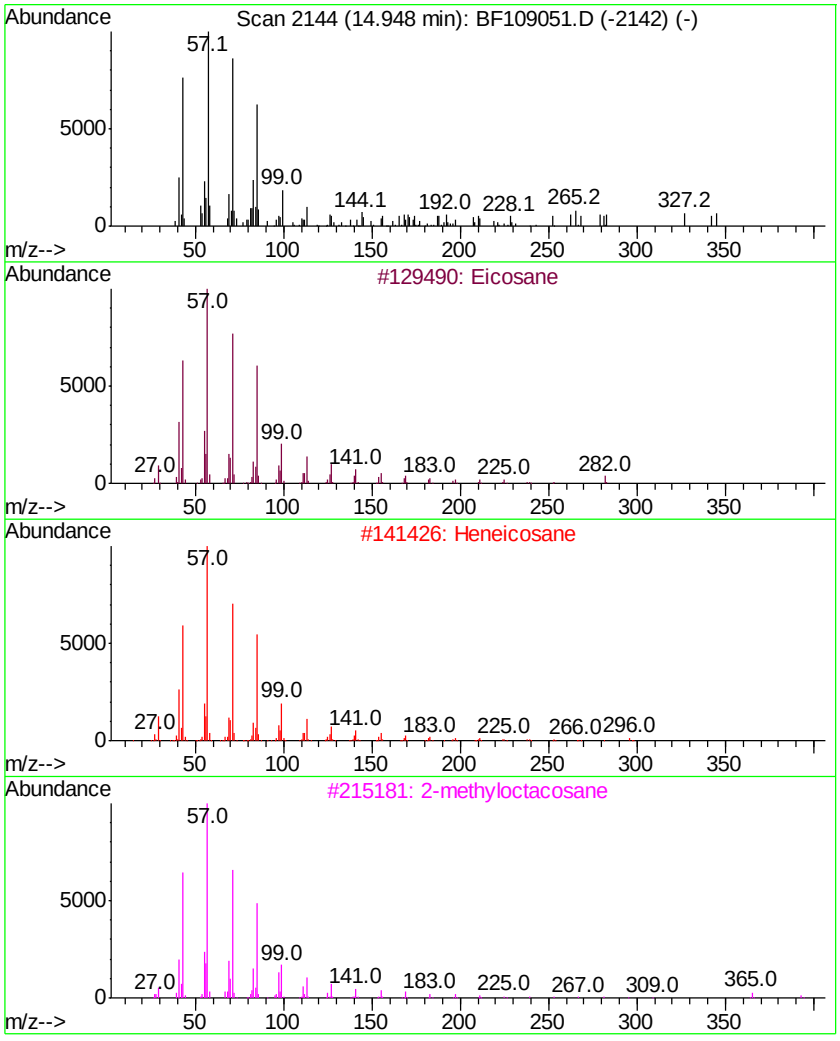
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

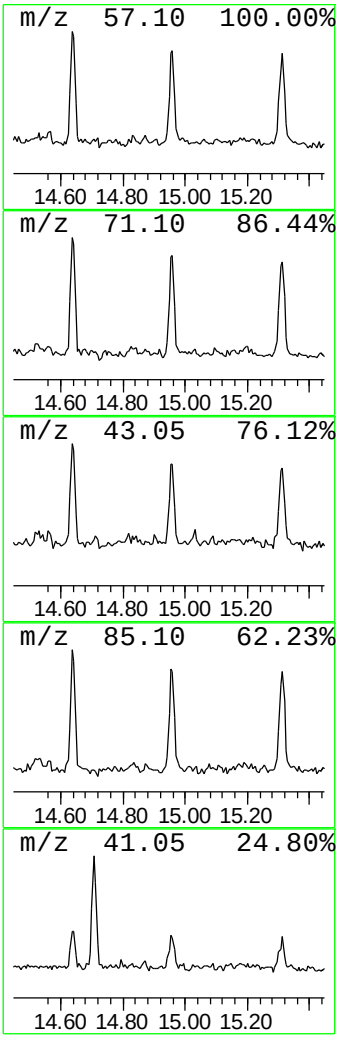
****

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.37 ng	94802	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SP-PIT-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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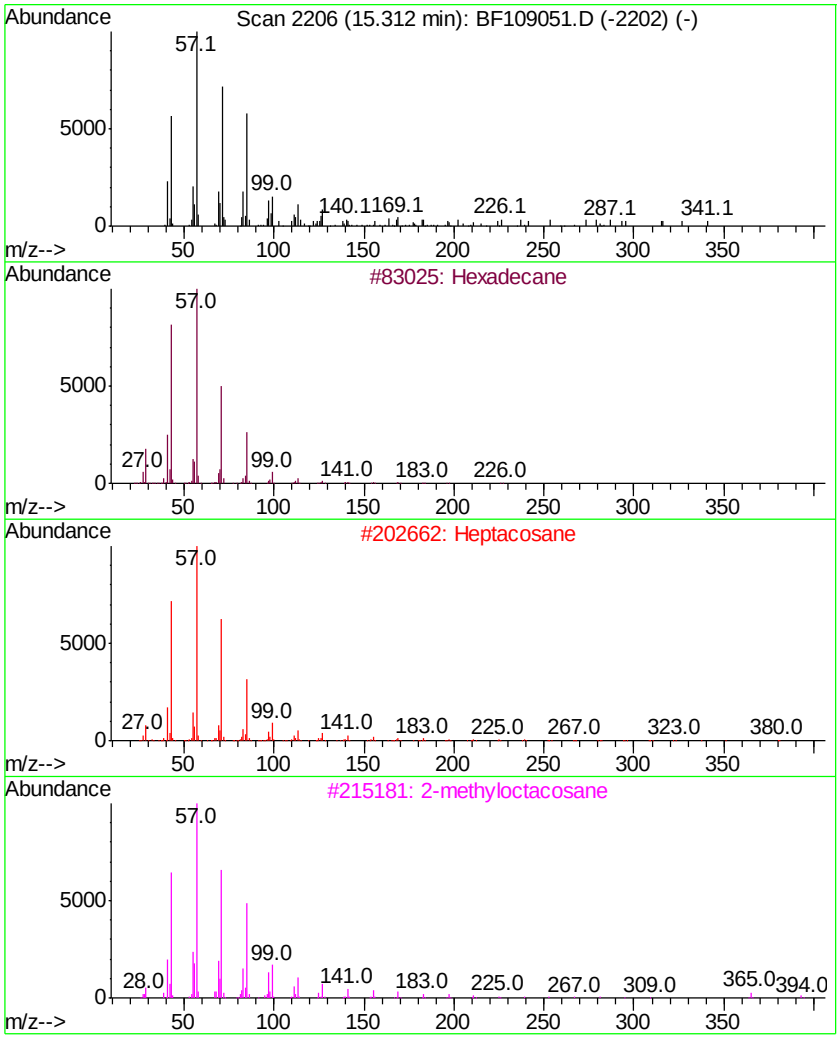
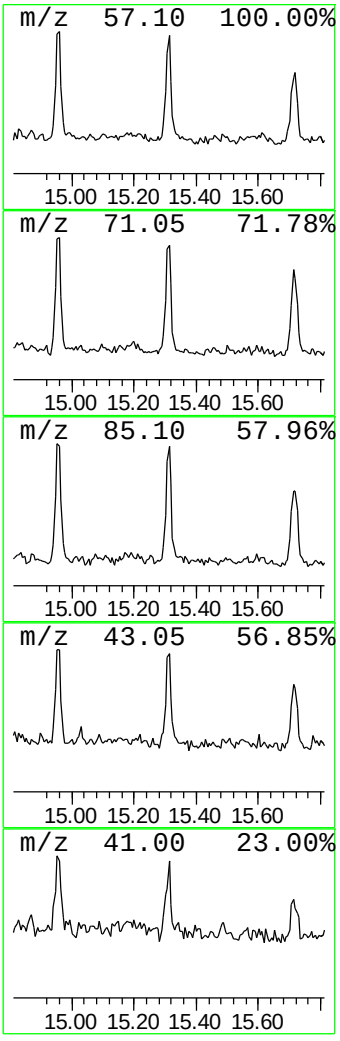
Peak Number 8 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.30 ng	91837	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Heptacosane	380	C27H56	000593-49-7	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	87





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.92	2.9	ng	129091	1	6.72	893761	20.0
unknown6.49	6.49	71.2	ng	3179880	1	6.72	893761	20.0
Sulfurous acid, o...	13.72	4.2	ng	198840	5	13.85	942557	20.0
Heneicosane	14.64	2.5	ng	98634	6	15.26	798556	20.0
Supraene	14.71	3.8	ng	152142	6	15.26	798556	20.0
Eicosane	14.95	2.4	ng	94802	6	15.26	798556	20.0
Hexadecane	15.31	2.3	ng	91837	6	15.26	798556	20.0