LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103118\
Data File : BF110339.D
Acq On : 31 Oct 2018 18:09
Operator : JU/SJ
Sample : J5730-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102918-TIPC-E-D-M

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-BF102318.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	2.299	29	36	46	rVB	1305688	1849401	65.52%	10.025%
2	5.199	526	529	543	rVB	36461	46087	1.63%	0.250%
3	5.593	593	596	613	rBV	688527	726405	25.74%	3.937%
4	6.593	762	766	778	rBV2	508695	531141	18.82%	2.879%
5	6.740	787	791	795	rBV	1569215	1402924	49.70%	7.604%
6	6.975	827	831	837	rBV	640823	541722	19.19%	2.936%
7	7.134	853	858	861	rBV	2038860	1952017	69.16%	10.581%
8	7.540	922	927	930	rBV	1633528	1547106	54.81%	8.386%
9	8.257	1045	1049	1054	rBV	715217	646539	22.91%	3.505%
10	9.334	1227	1232	1235	rBV	3310124	2822561	100.00%	15.300%
11	10.022	1345	1349	1361	rVB	737567	760878	26.96%	4.124%
12	10.810	1479	1483	1495	rBV	1027929	1072261	37.99%	5.812%
13	11.516	1599	1603	1616	rBV	772278	703880	24.94%	3.815%
14	13.098	1868	1872	1876	rBV	2143667	2066339	73.21%	11.201%
15	13.980	2018	2022	2027	rBV2	41593	57156	2.02%	0.310%
16	14.169	2050	2054	2062	rBV	485021	487269	17.26%	2.641%
17	14.292	2072	2075	2080	rBV	40082	40433	1.43%	0.219%
18	14.598	2124	2127	2132	rBV	72717	66767	2.37%	0.362%
19	14.921	2179	2182	2187	rVB	108746	113951	4.04%	0.618%
20	15.280	2239	2243	2248	rBV	118892	134520	4.77%	0.729%
21	15.686	2307	2312	2313	rBV	124725	163334	5.79%	0.885%
22	15.710	2313	2316	2325	rVB	296211	403882	14.31%	2.189%
23	16.151	2385	2391	2398	rBV	107283	185075	6.56%	1.003%
24	16.686	2477	2482	2488	rBV	71744	126970	4.50%	0.688%

Sum of corrected areas: 18448618

LSC Report - Integrated Chromatogram

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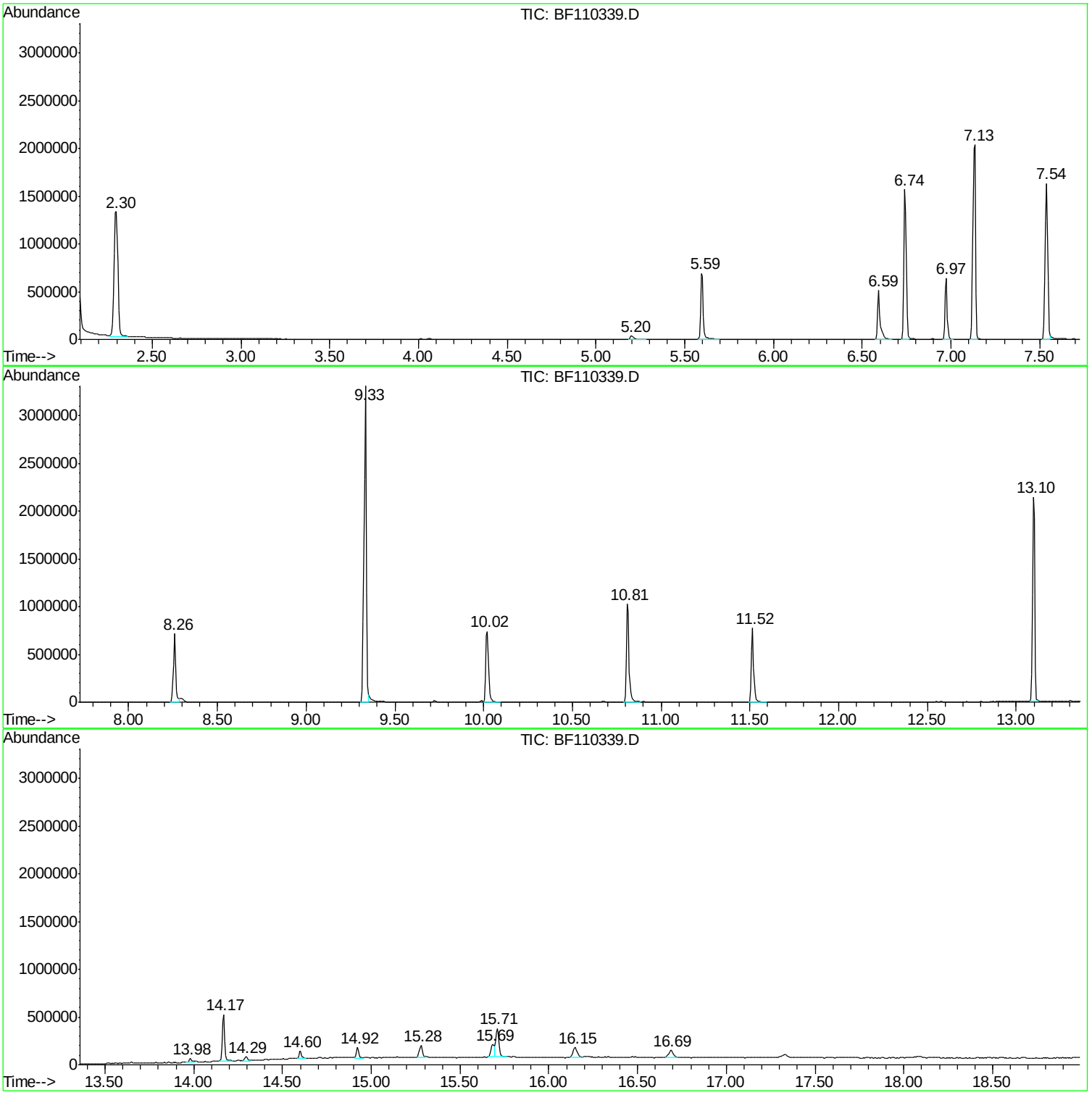
Sample : J5730-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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

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Data File : BF110339.D
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Operator : JU/SJ
Sample : J5730-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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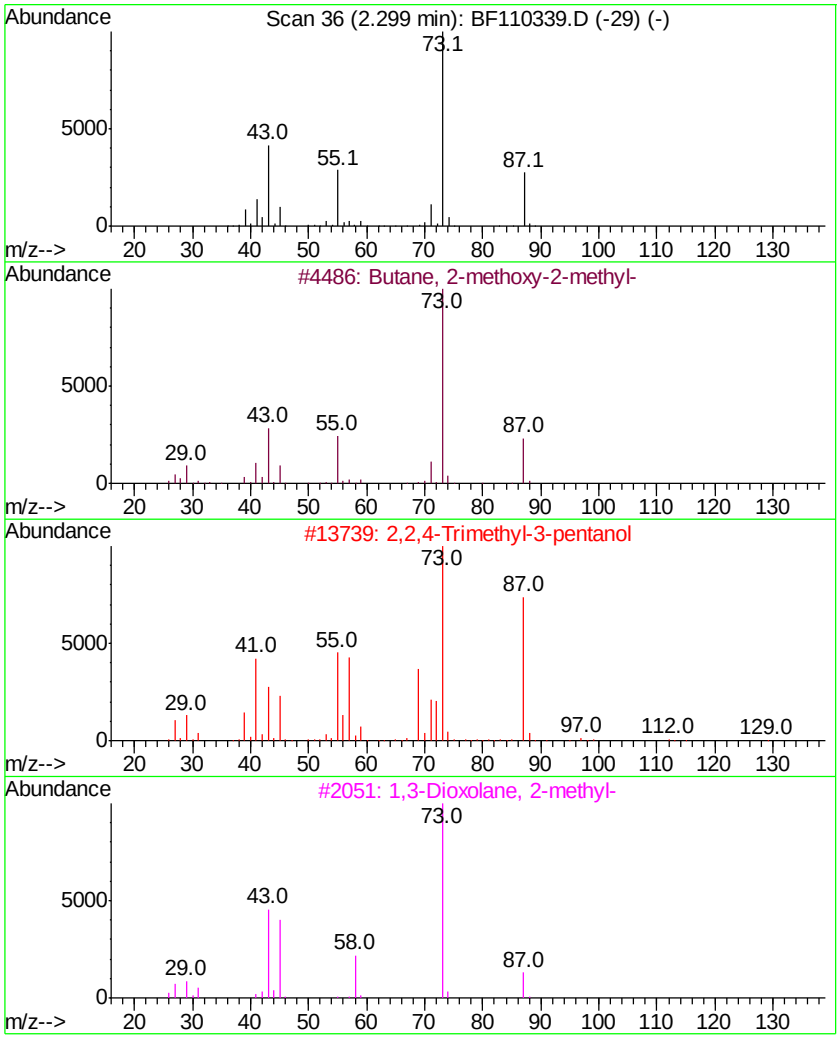
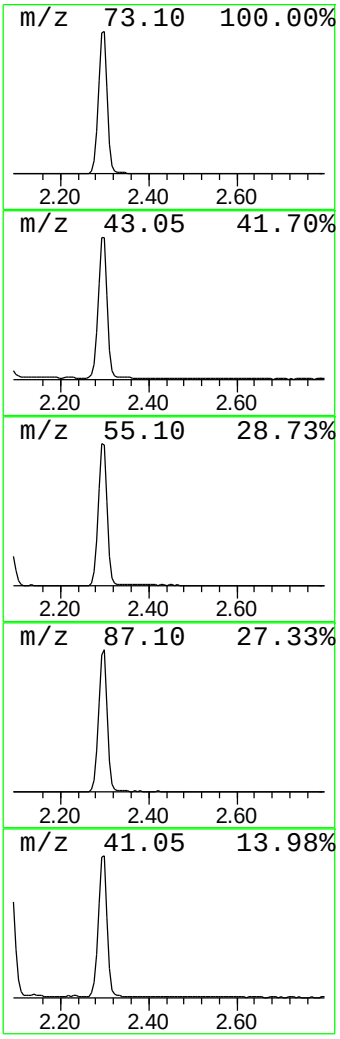
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	68.28 ng	1849400	1,4-Dichlorobenzene-d4	6.97

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Library Search Compound Report

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Operator : JU/SJ
Sample : J5730-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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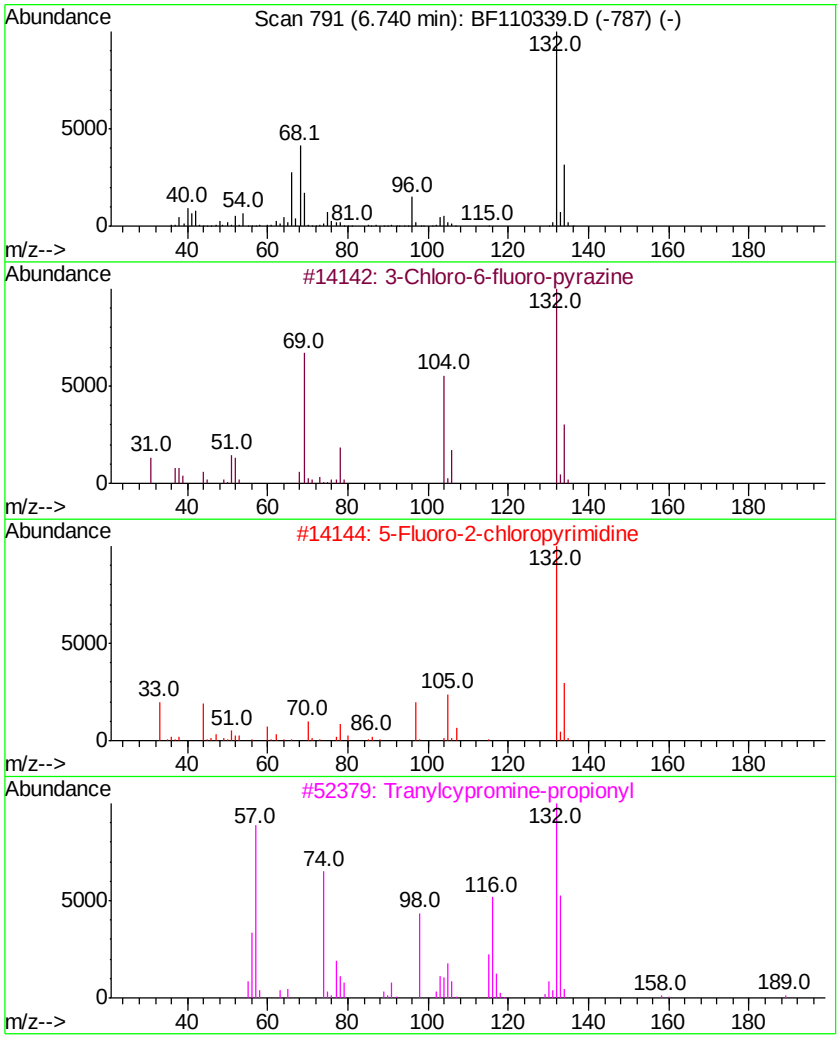
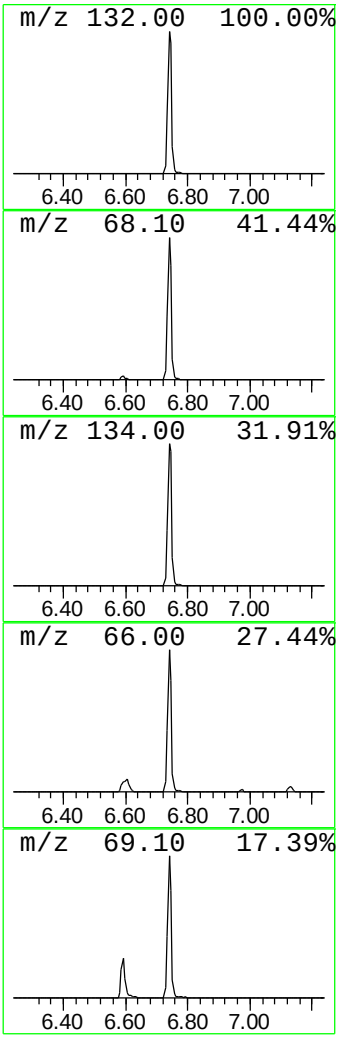
Peak Number 2 unknown6.74 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	51.80 ng	1402920	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103118\
Data File : BF110339.D
Acq On : 31 Oct 2018 18:09
Operator : JU/SJ
Sample : J5730-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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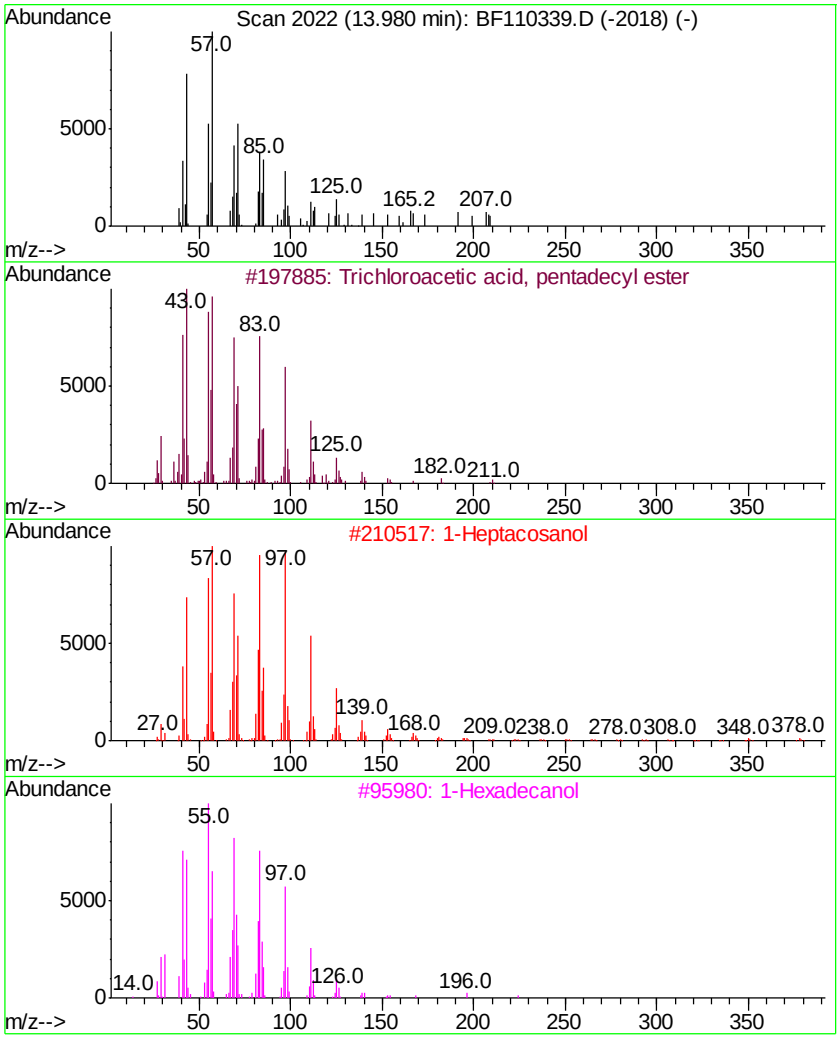
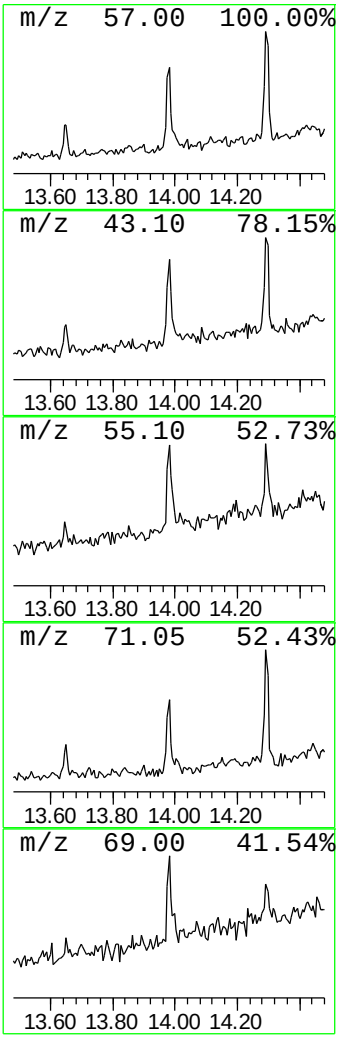
Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	2.35 ng	57156	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	58
2	1-Heptacosanol	396	C27H56O	002004-39-9	53
3	1-Hexadecanol	242	C16H34O	036653-82-4	53
4	Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	53
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	53





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Data File : BF110339.D
Acq On : 31 Oct 2018 18:09
Operator : JU/SJ
Sample : J5730-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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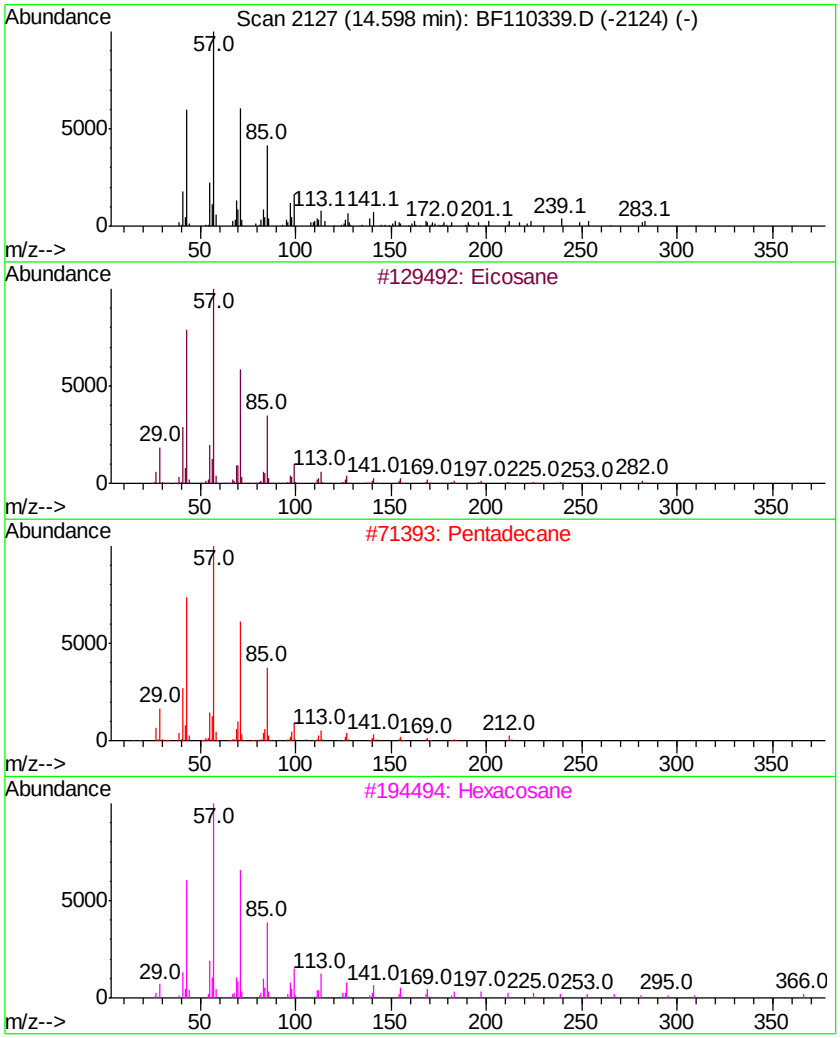
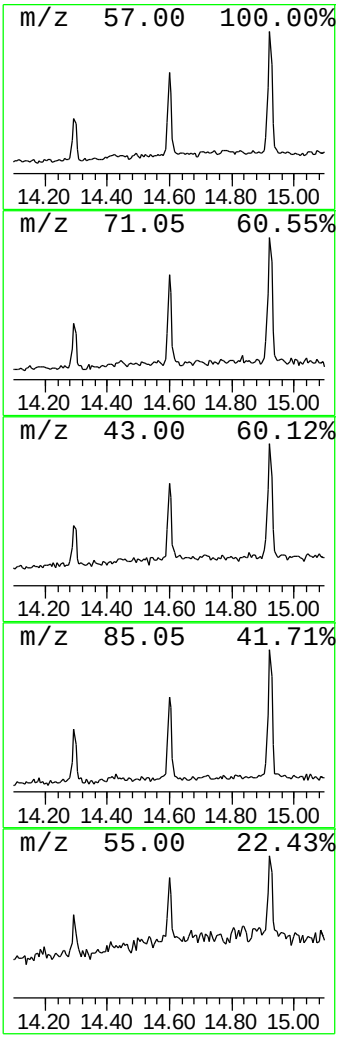
Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.74 ng	66767	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Pentadecane	212	C15H32	000629-62-9	81
3	Hexacosane	366	C26H54	000630-01-3	80
4	Tetracosane	338	C24H50	000646-31-1	80
5	Heneicosane	296	C21H44	000629-94-7	74





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Data File : BF110339.D
Acq On : 31 Oct 2018 18:09
Operator : JU/SJ
Sample : J5730-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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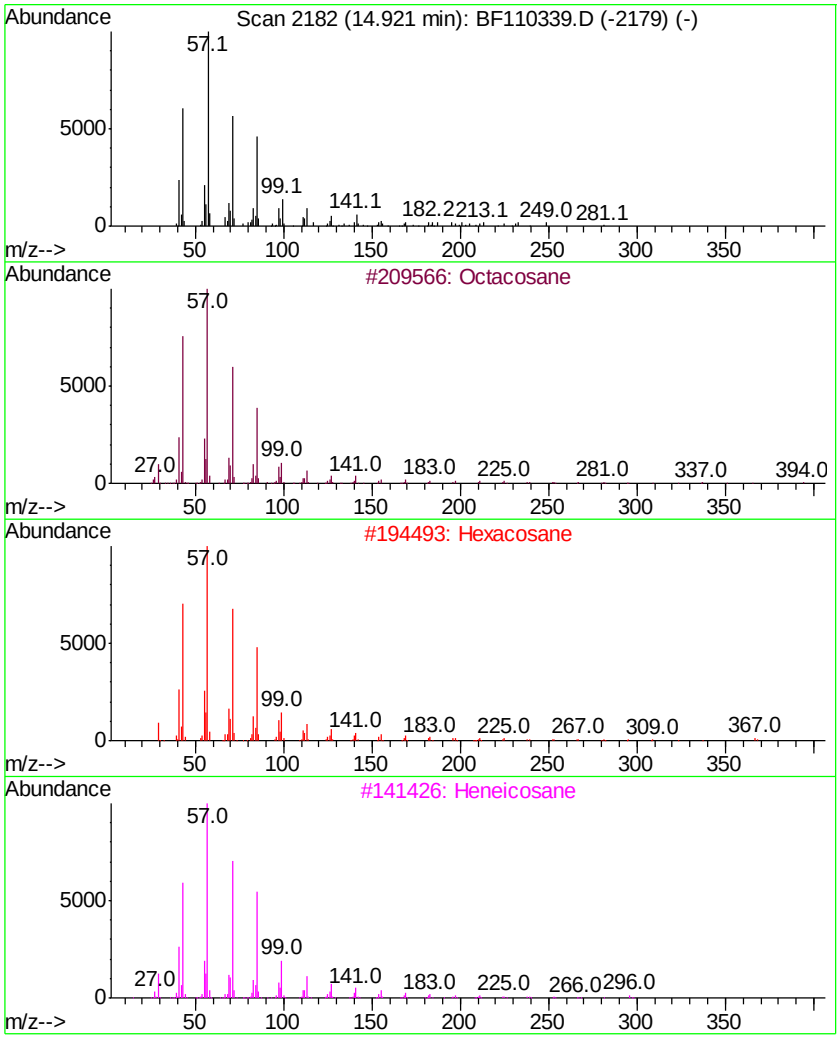
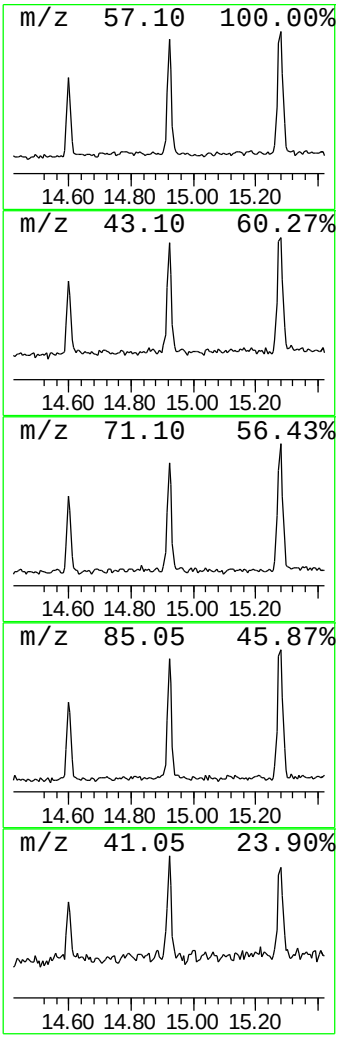
Peak Number 6 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.68 ng	113951	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentadecane	212	C15H32	000629-62-9	83





Library Search Compound Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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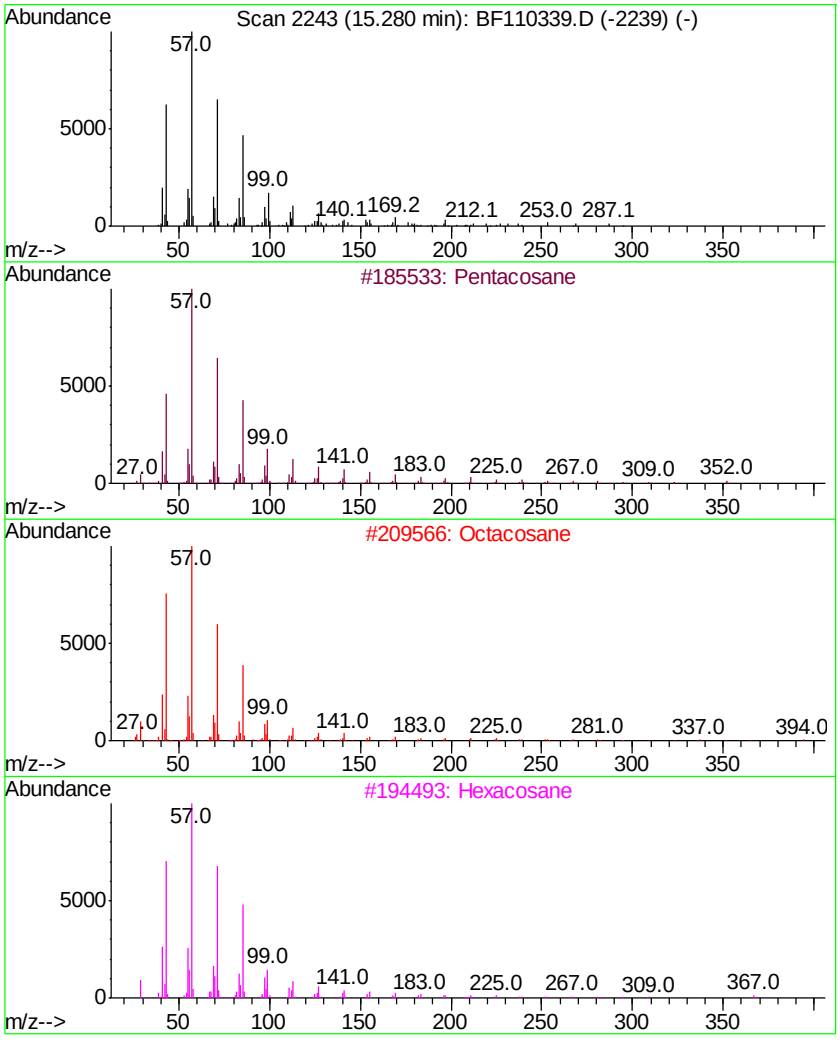
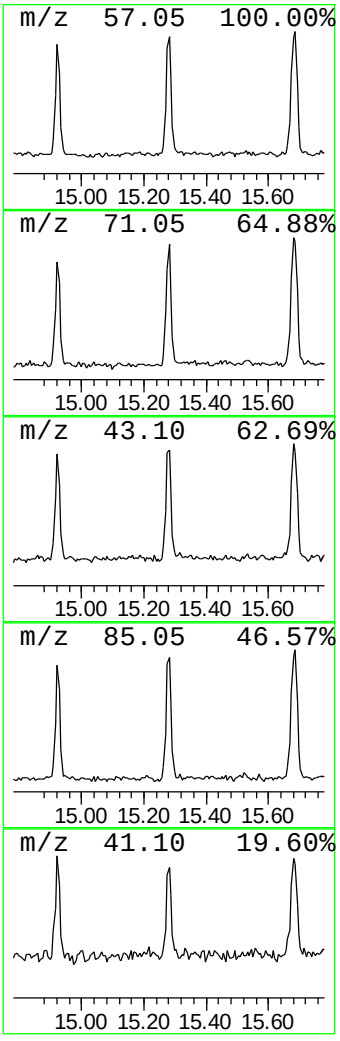
Peak Number 7 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	6.66 ng	134520	Perylene-d12	15.71

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	Hexacosane	366	C26H54	000630-01-3	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Hentriacontane	437	C31H64	000630-04-6	87





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ClientSampleId : 102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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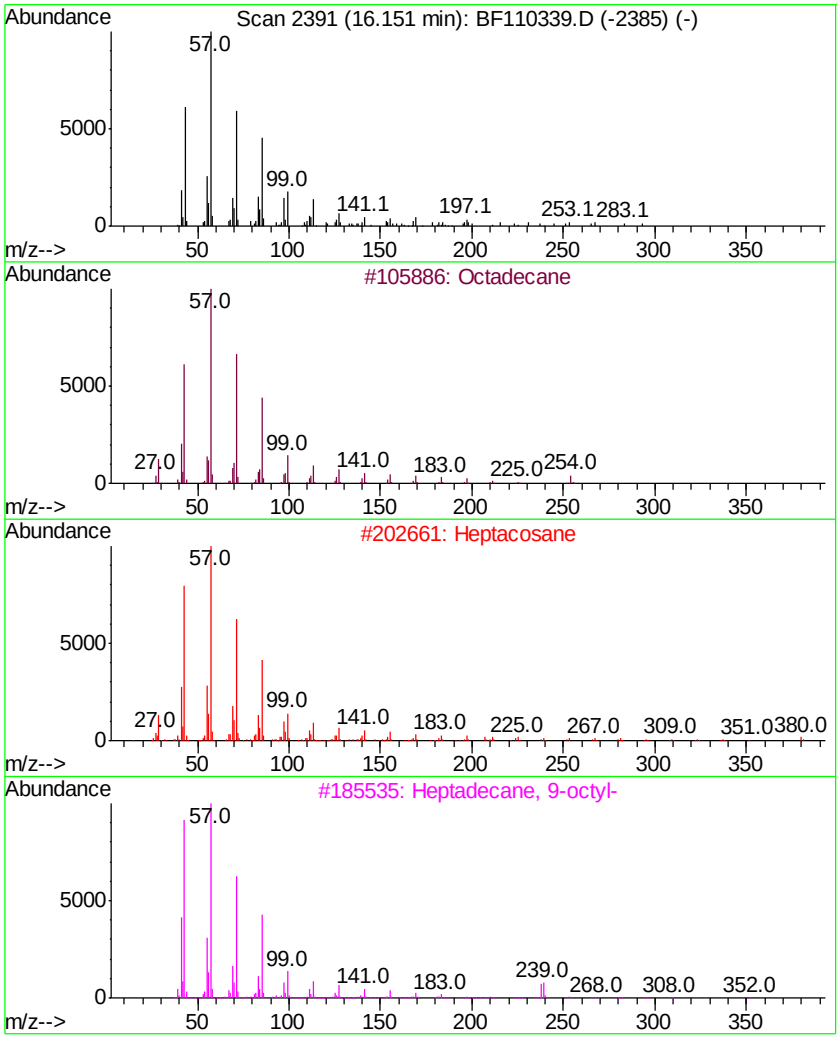
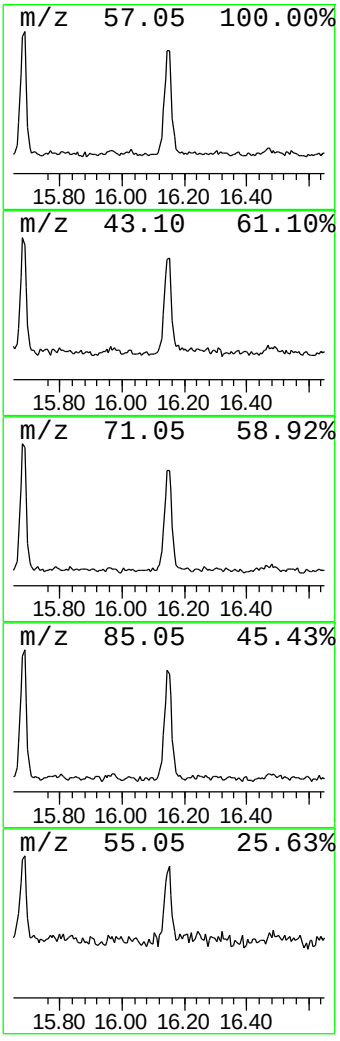
Peak Number 8 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	9.16 ng	185075	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	87
2	Heptacosane	380	C27H56	000593-49-7	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	87





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TIC Integration Parameters: LSCINT.P

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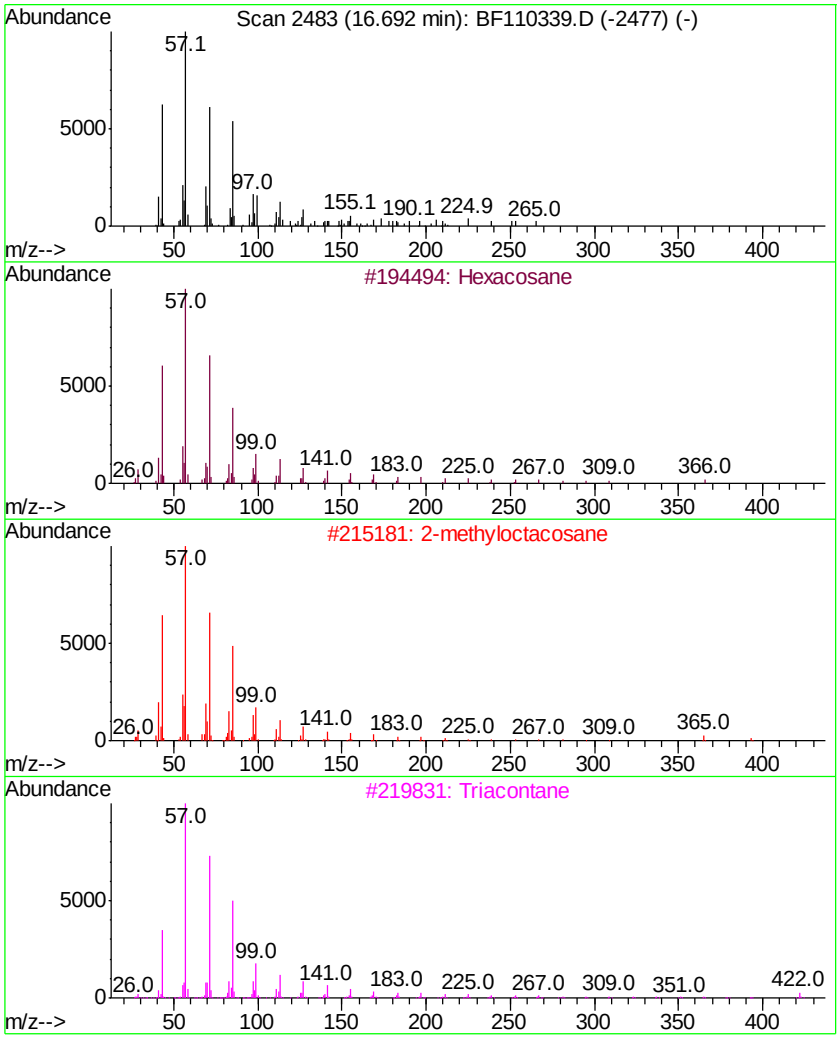
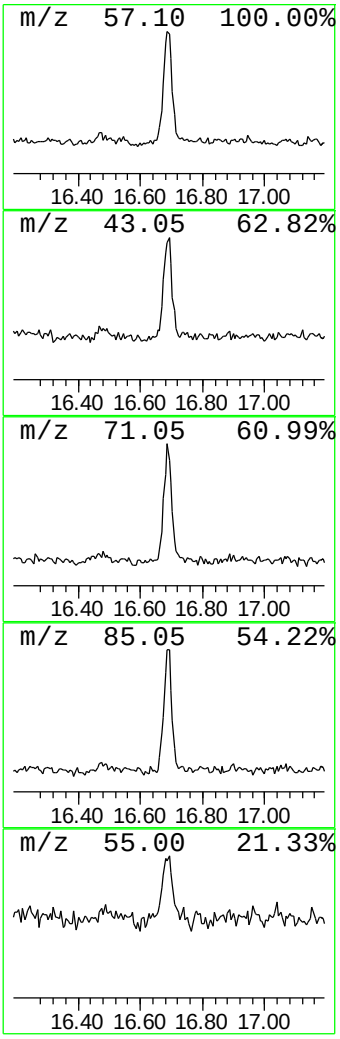
Peak Number 9 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	6.29 ng	126970	Perylene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
5	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	90





Tentatively Identified Compound (LSC) summary

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ClientSampleId : 102918-TIPC-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.30	68.3	ng	1849400	1	6.97	541722	20.0
unknown6.74	6.74	51.8	ng	1402920	1	6.97	541722	20.0
Trichloroacetic a...	13.98	2.4	ng	57156	5	14.17	487269	20.0
Eicosane	14.60	2.7	ng	66767	5	14.17	487269	20.0
Octacosane	14.92	4.7	ng	113951	5	14.17	487269	20.0
Pentacosane	15.28	6.7	ng	134520	6	15.71	403882	20.0
Octadecane	16.15	9.2	ng	185075	6	15.71	403882	20.0
Hexacosane	16.69	6.3	ng	126970	6	15.71	403882	20.0