LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110771.D
Acq On : 14 Nov 2018 18:22
Operator : JU/SJ
Sample : J5889-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-E

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	2.252	23	28	37	rVB	100959	145580	6.37%	0.782%
2	5.187	523	527	542	rBV	56982	94199	4.12%	0.506%
3	5.569	587	592	612	rBV	1971385	2019549	88.32%	10.844%
4	6.575	758	763	782	rBV	1955905	2250438	98.42%	12.083%
5	6.716	782	787	790	rBV	2419394	2144263	93.77%	11.513%
6	6.945	822	826	832	rBV	441715	410911	17.97%	2.206%
7	7.098	848	852	872	rBV	1872713	1636259	71.56%	8.786%
8	7.510	918	922	937	rBV	1356323	1358212	59.40%	7.293%
9	8.222	1040	1043	1062	rBV	481844	546820	23.91%	2.936%
10	9.298	1222	1226	1229	rBV	2638056	2286629	100.00%	12.278%
11	9.692	1289	1293	1300	rBV	201017	201313	8.80%	1.081%
12	9.980	1339	1342	1354	rBV	589691	606397	26.52%	3.256%
13	10.774	1473	1477	1490	rBV	1276074	1356498	59.32%	7.284%
14	11.480	1593	1597	1605	rBV	524920	559705	24.48%	3.005%
15	11.980	1679	1682	1690	rBV3	18856	26007	1.14%	0.140%
16	13.063	1861	1866	1869	rBV	1759721	1715425	75.02%	9.211%
17	13.933	2011	2014	2023	rBV	54481	69117	3.02%	0.371%
18	14.127	2043	2047	2056	rBV	454210	441752	19.32%	2.372%
19	14.557	2116	2120	2123	rBV	28791	35455	1.55%	0.190%
20	14.868	2170	2173	2177	rVB2	43116	44369	1.94%	0.238%
21	15.221	2229	2233	2242	rVB	46200	56978	2.49%	0.306%
22	15.615	2296	2300	2303	rBV	50948	65311	2.86%	0.351%
23	15.657	2303	2307	2320	rVB	275052	415199	18.16%	2.229%
24	16.068	2372	2377	2382	rBV2	49867	80411	3.52%	0.432%
25	16.592	2462	2466	2471	rVB2	30842	57369	2.51%	0.308%

Sum of corrected areas: 18624166

LSC Report - Integrated Chromatogram

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Sample : J5889-05
Misc :
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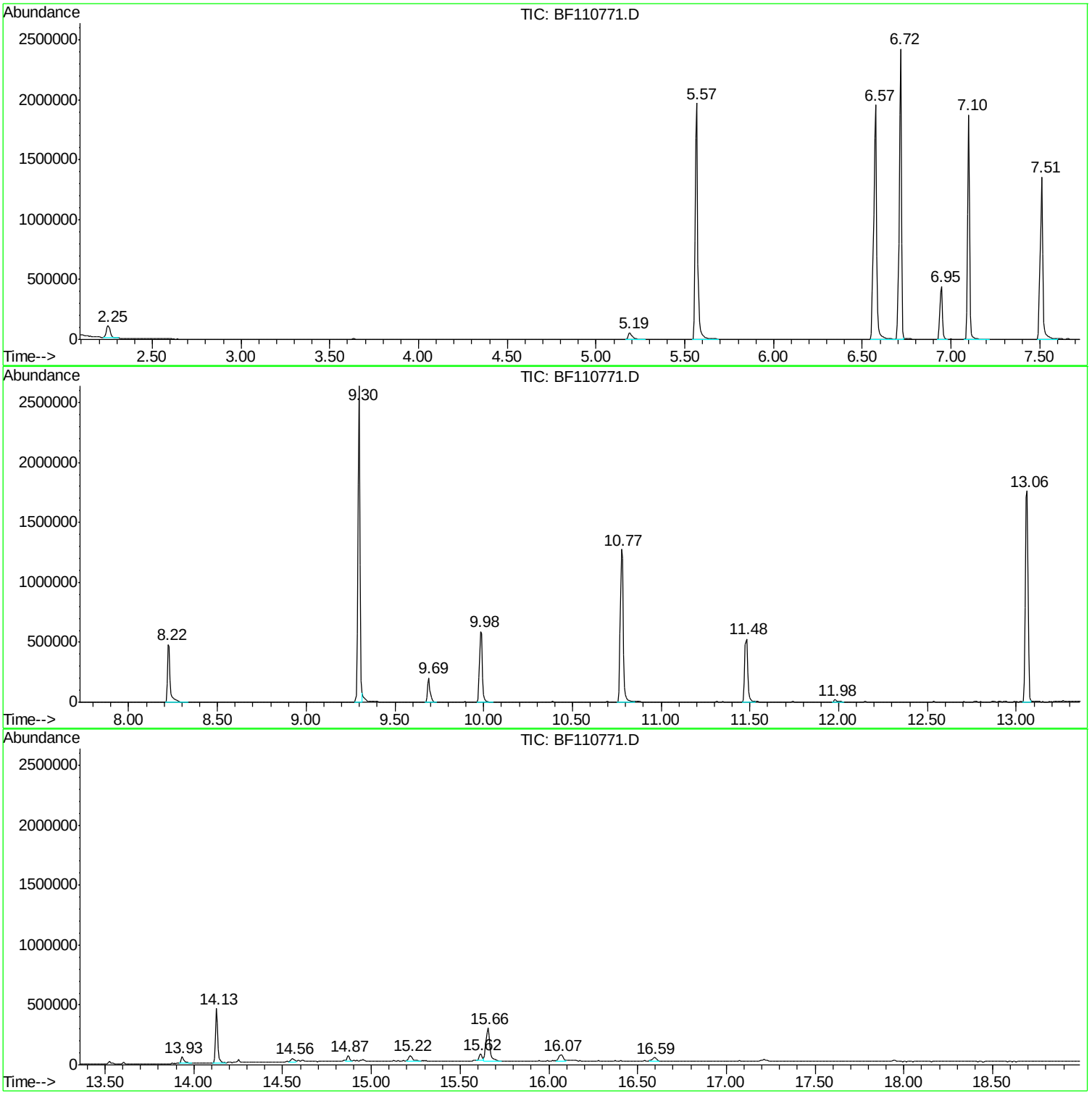
Instrument : BNA_F
ClientSampleId : WALL-E

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\BF111418\
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
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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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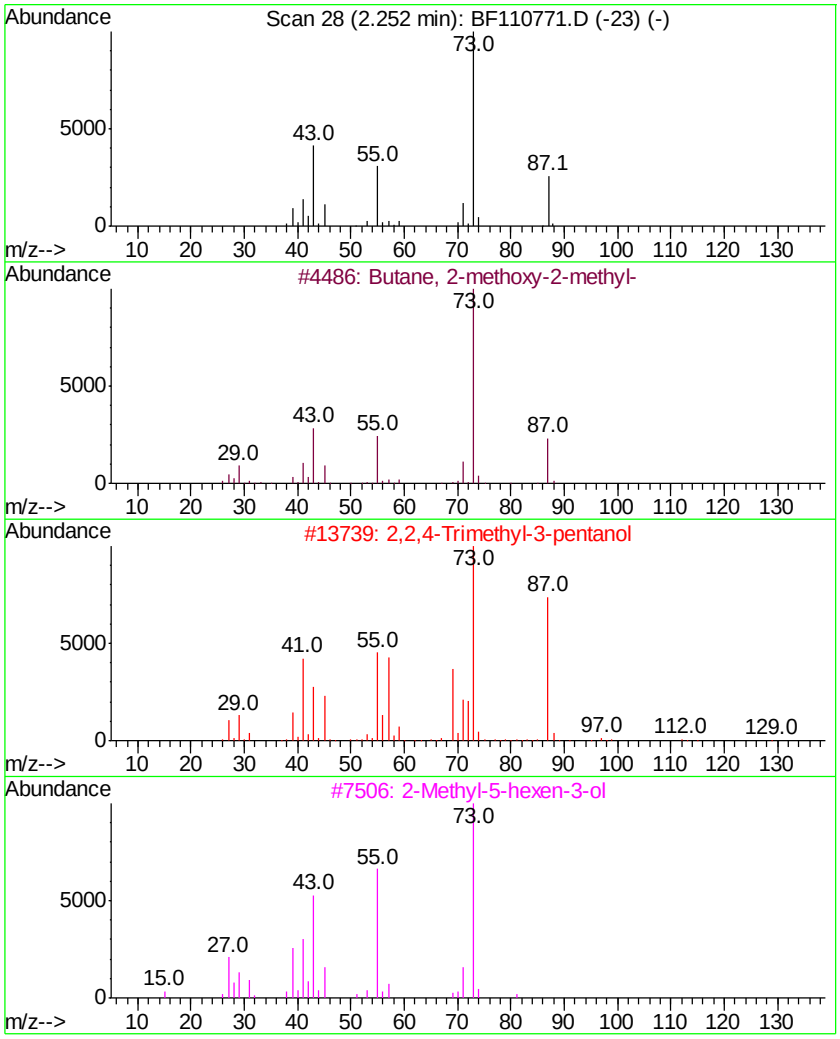
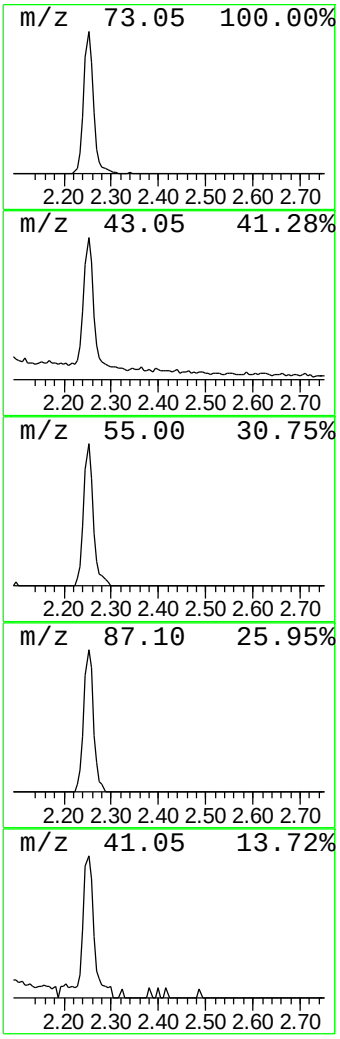
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	7.09 ng	145580	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	39
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





Library Search Compound Report

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Operator : JU/SJ
Sample : J5889-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-E

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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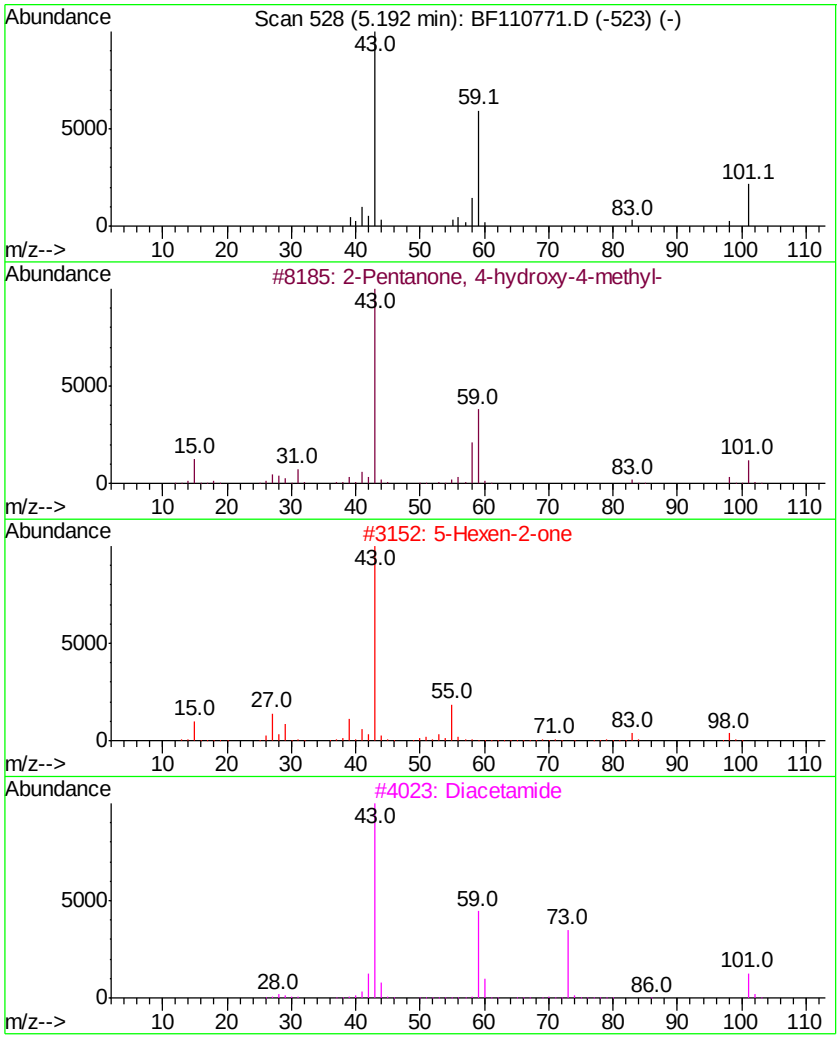
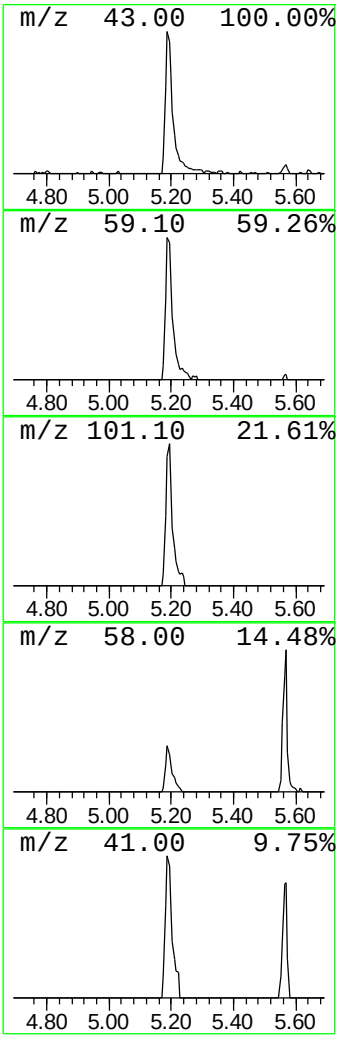
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	4.58 ng	94199	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	3-Octanol	130	C8H18O	000589-98-0	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Library Search Compound Report

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Data File : BF110771.D
Acq On : 14 Nov 2018 18:22
Operator : JU/SJ
Sample : J5889-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-E

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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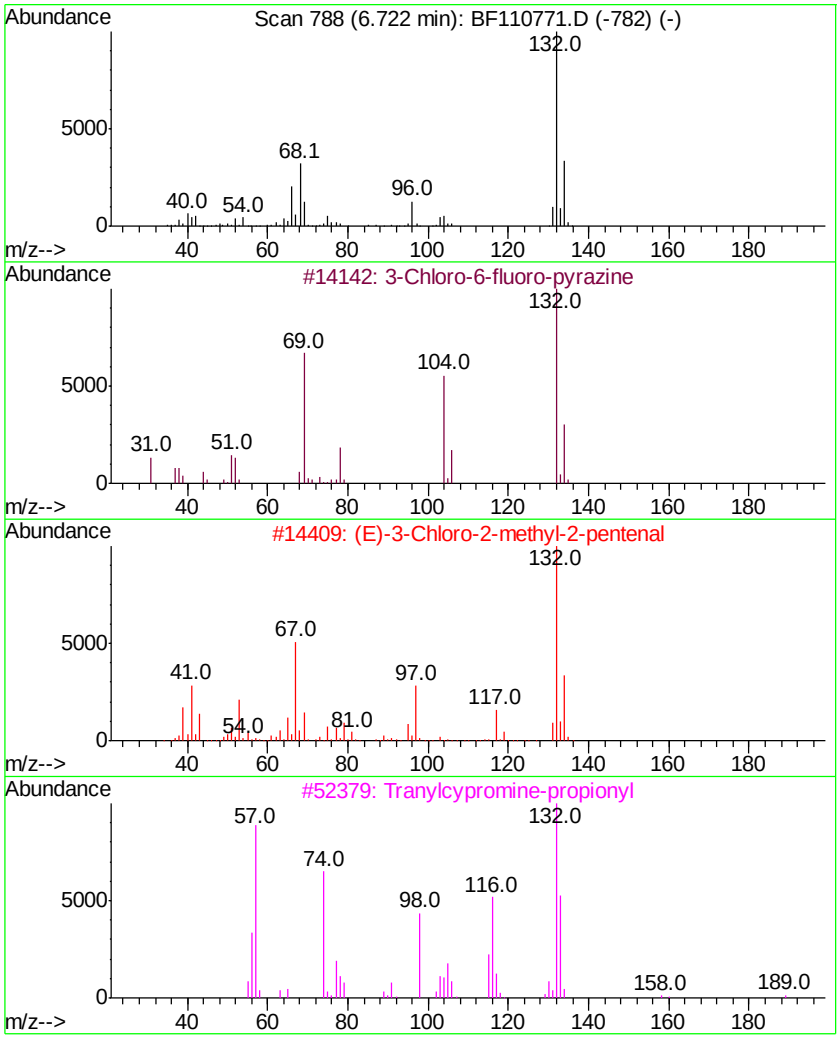
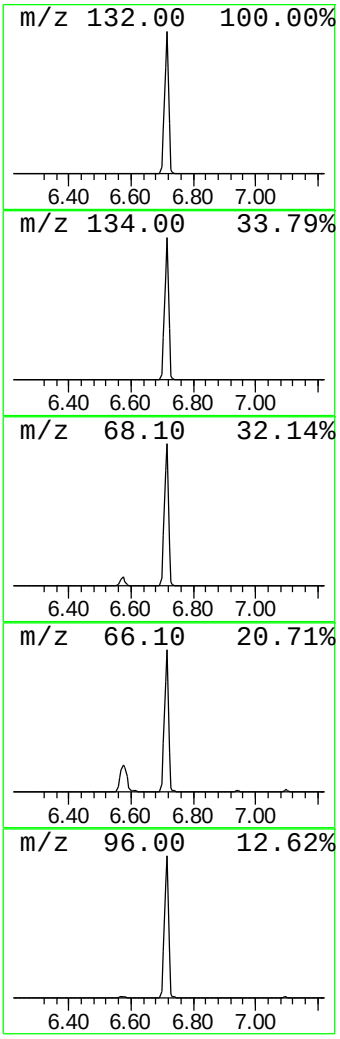
Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	104.37 ng	2144260	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
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Operator : JU/SJ
Sample : J5889-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-E

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
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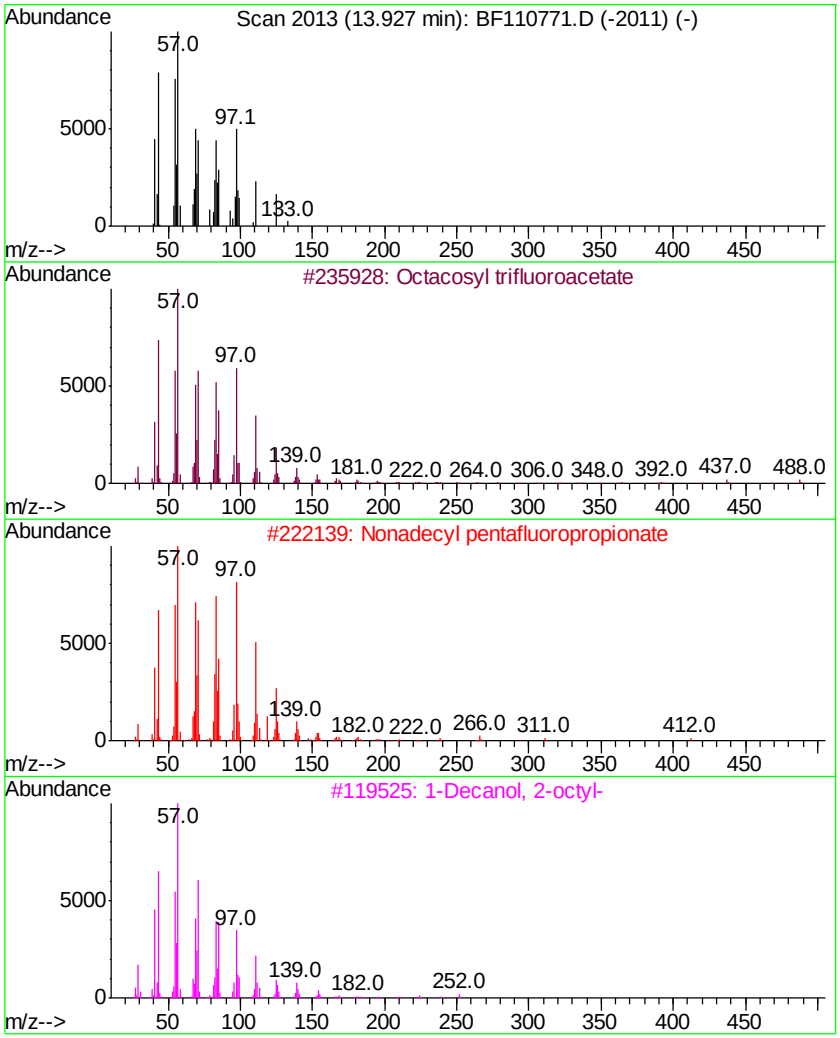
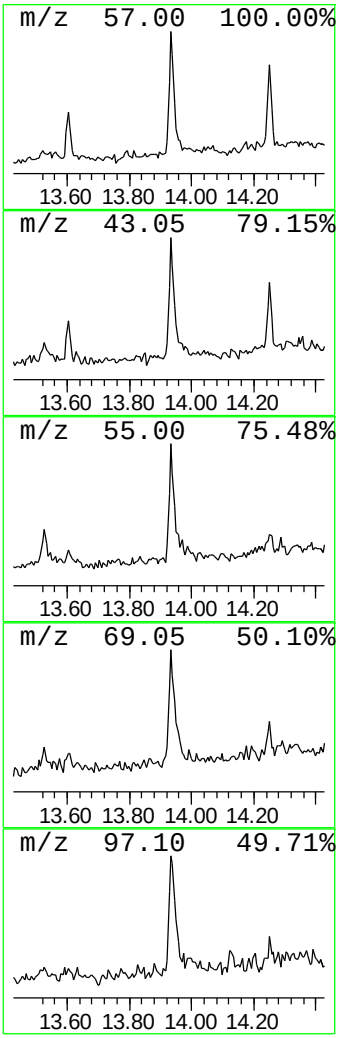
Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.13 ng	69117	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	91
4	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	91





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Operator : JU/SJ
Sample : J5889-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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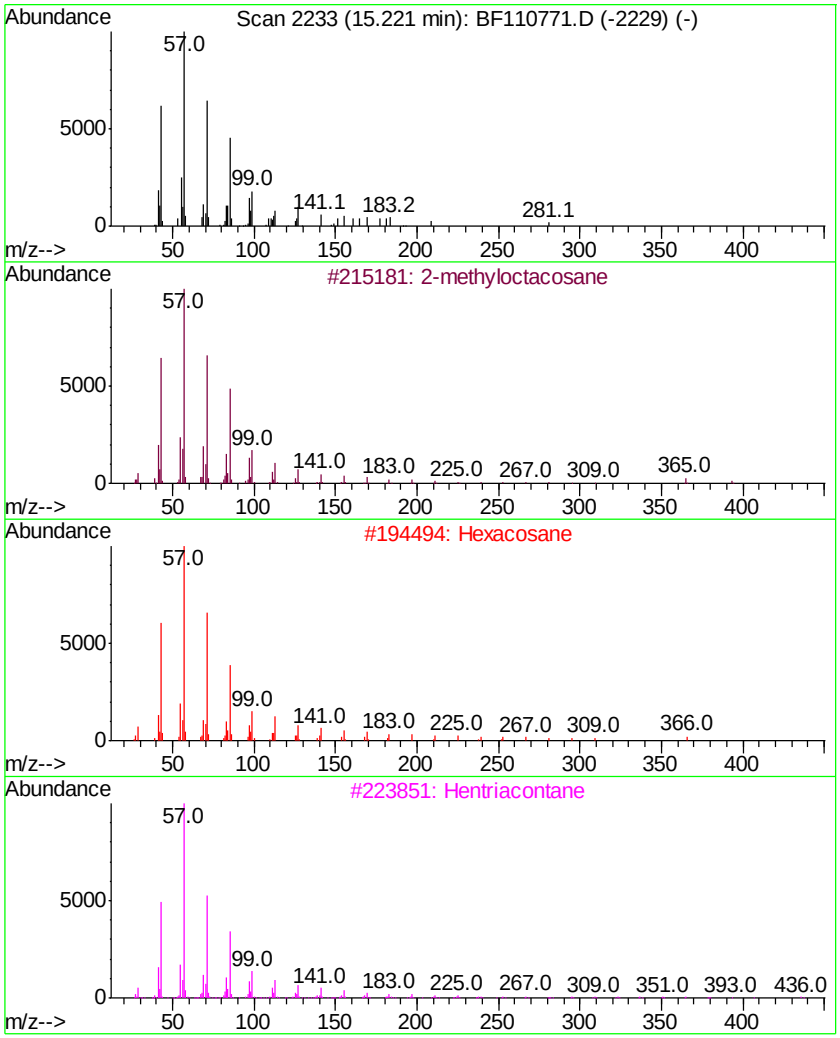
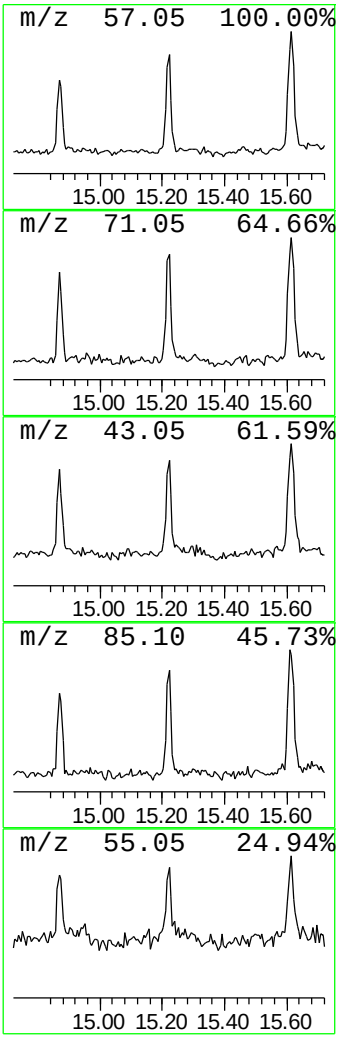
Peak Number 7 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.74 ng	56978	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Hentriacontane	437	C31H64	000630-04-6	86
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
5	Hexadecane	226	C16H34	000544-76-3	80





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Sample : J5889-05
Misc :
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Instrument : BNA_F
ClientSampleId : WALL-E

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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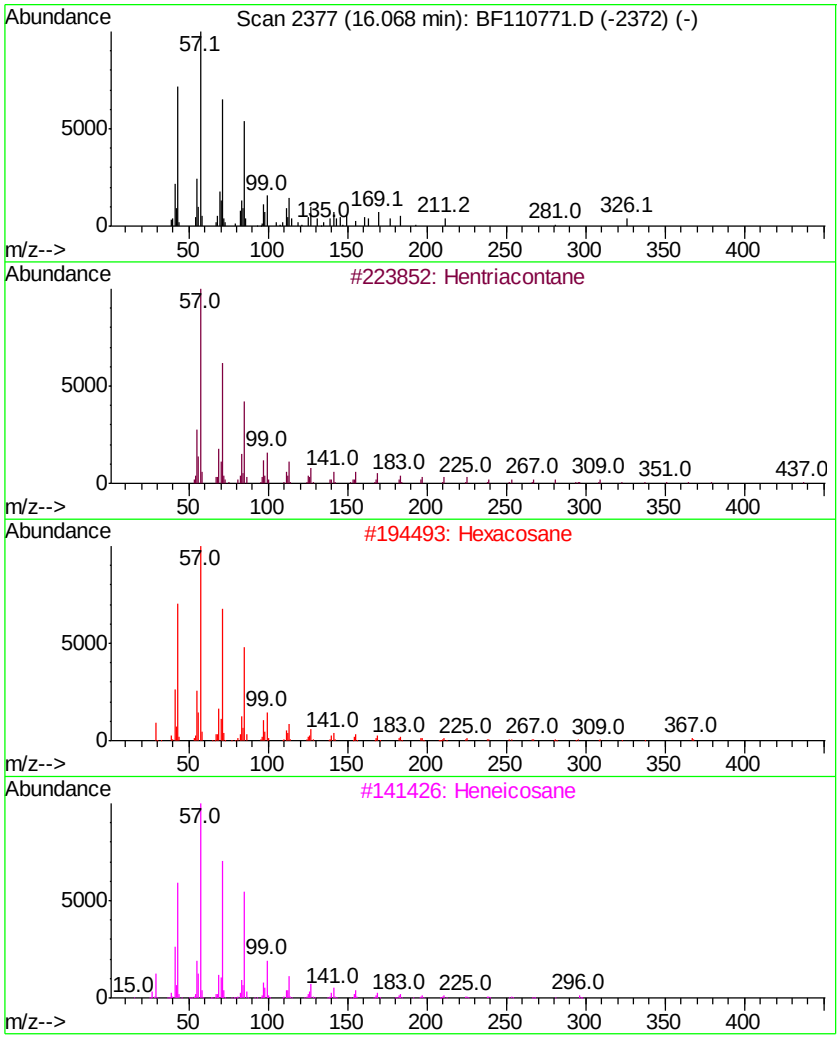
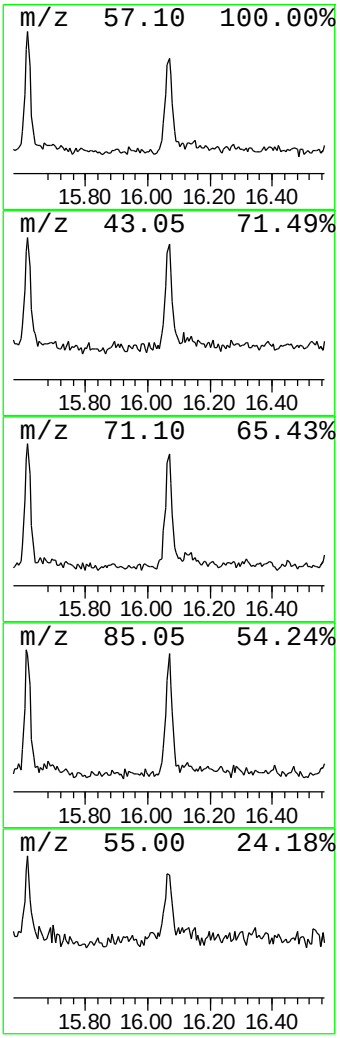
Peak Number 8 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	3.87 ng	80411	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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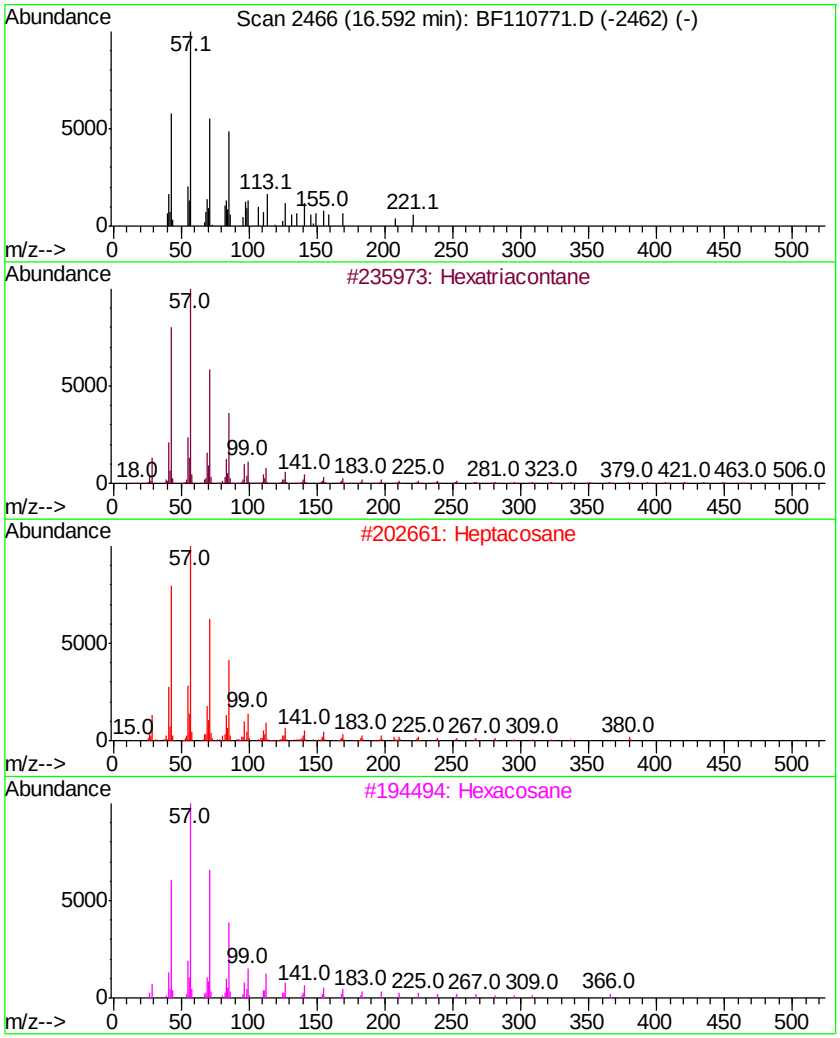
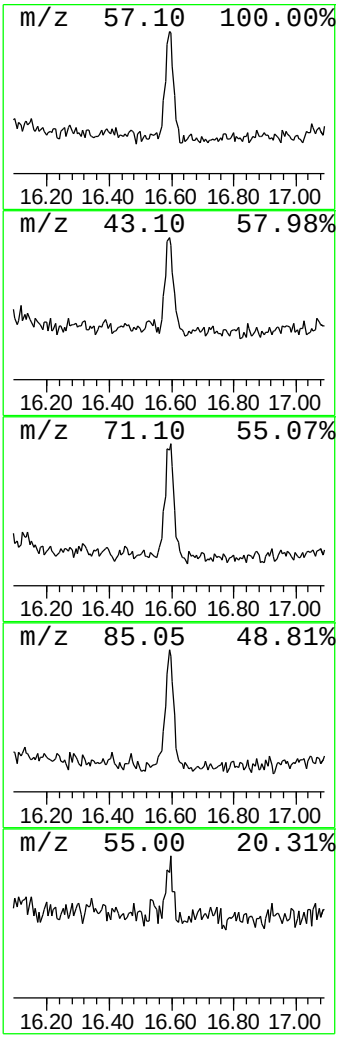
Peak Number 9 Hexatriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	2.76 ng	57369	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	86
2	Heptacosane	380	C27H56	000593-49-7	72
3	Hexacosane	366	C26H54	000630-01-3	72
4	Hentriacontane	437	C31H64	000630-04-6	72
5	Triacontane	422	C30H62	000638-68-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111418\
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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...	2.25	7.1	ng	145580	1	6.95	410911	20.0
2-Pentanone, 4-hy...	5.19	4.6	ng	94199	1	6.95	410911	20.0
unknown6.72	6.72	104.4	ng	2144260	1	6.95	410911	20.0
Octacosyl trifluo...	13.93	3.1	ng	69117	5	14.13	441752	20.0
2-methyloctacosane	15.22	2.7	ng	56978	6	15.66	415199	20.0
Hentriacontane	16.07	3.9	ng	80411	6	15.66	415199	20.0
Hexatriacontane	16.59	2.8	ng	57369	6	15.66	415199	20.0