LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117364.D
Acq On : 10 Oct 2019 17:08
Operator : JU
Sample : K5297-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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-BF091319.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	5.004	493	496	507	rBV	36304	55330	5.42%	0.606%
2	5.422	563	567	592	rBV	651819	827928	81.09%	9.075%
3	6.439	736	740	758	rBV	828278	928588	90.95%	10.178%
4	6.569	758	762	778	rVB	1088001	956329	93.67%	10.482%
5	6.792	797	800	817	rVB	252686	242306	23.73%	2.656%
6	6.951	823	827	844	rBV	746459	689954	67.58%	7.562%
7	7.357	892	896	920	rBV	449324	548852	53.76%	6.016%
8	8.075	1015	1018	1033	rBV	232825	304732	29.85%	3.340%
9	9.151	1197	1201	1220	rBV	1023124	1021002	100.00%	11.191%
10	9.545	1265	1268	1278	rBV	108483	108823	10.66%	1.193%
11	9.828	1313	1316	1329	rBV	373704	375289	36.76%	4.113%
12	10.622	1447	1451	1467	rBV	558101	596684	58.44%	6.540%
13	11.316	1566	1569	1578	rBV	331272	371981	36.43%	4.077%
14	11.839	1655	1658	1670	rBV2	29959	42459	4.16%	0.465%
15	12.533	1773	1776	1782	rBV	15590	20488	2.01%	0.225%
16	12.763	1811	1815	1821	rBV	16994	22052	2.16%	0.242%
17	12.898	1834	1838	1846	rBV	1114884	980104	95.99%	10.742%
18	13.792	1986	1990	2003	rBV5	43263	87850	8.60%	0.963%
19	13.963	2015	2019	2029	rVB	278937	306065	29.98%	3.355%
20	14.110	2040	2044	2047	rBV2	18542	17496	1.71%	0.192%
21	14.415	2092	2096	2098	rBV	28382	25660	2.51%	0.281%
22	14.715	2141	2147	2151	rBV2	49678	72694	7.12%	0.797%
23	15.039	2198	2202	2207	rVB	64708	78972	7.73%	0.866%
24	15.415	2260	2266	2278	rVB2	200623	314942	30.85%	3.452%
25	15.827	2331	2336	2341	rVB	43811	66608	6.52%	0.730%
26	16.309	2412	2418	2424	rVB3	24786	44671	4.38%	0.490%
27	16.886	2512	2516	2521	rVB8	8271	15797	1.55%	0.173%

Sum of corrected areas: 9123656

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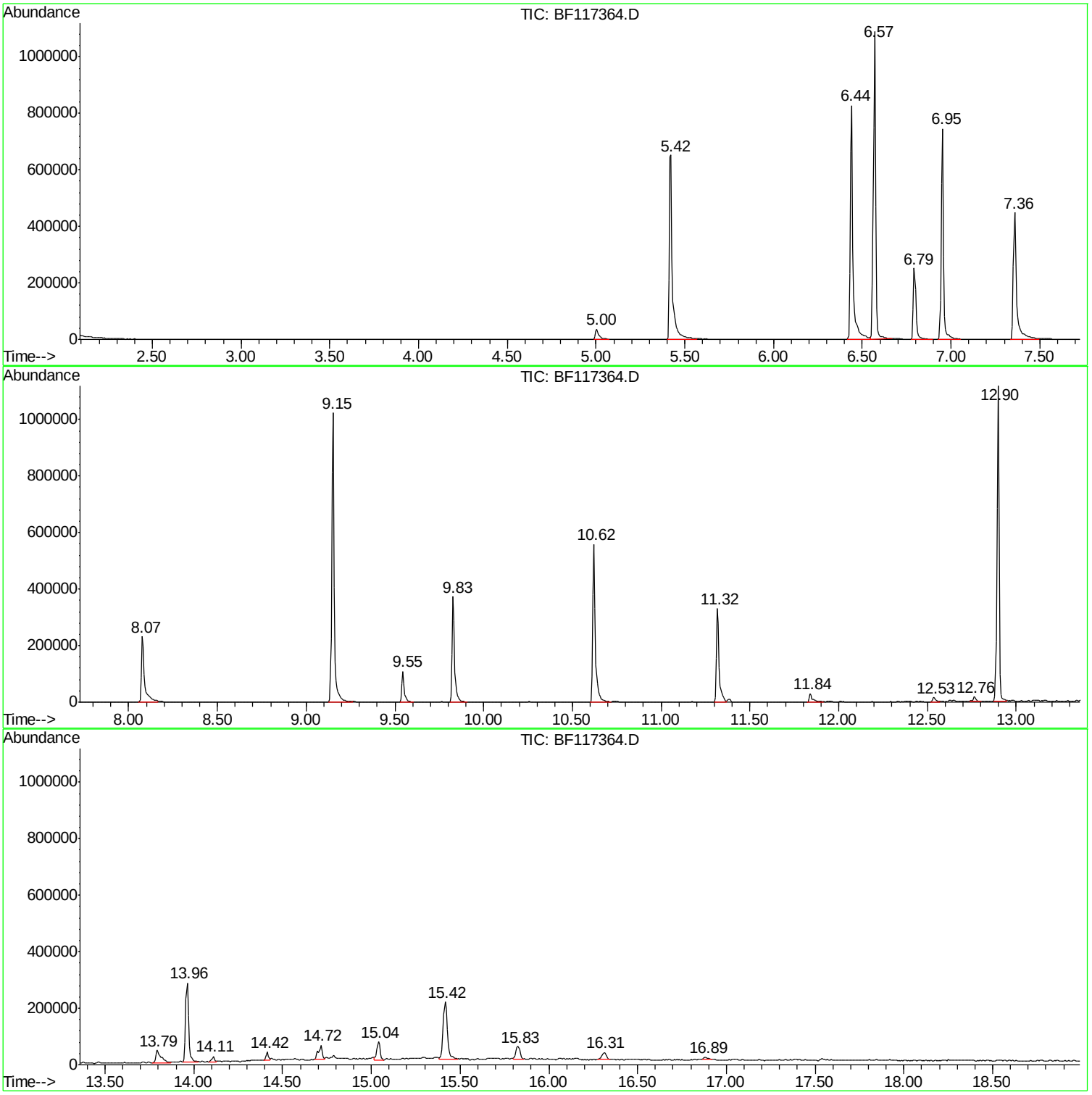
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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Instrument : BNA_F
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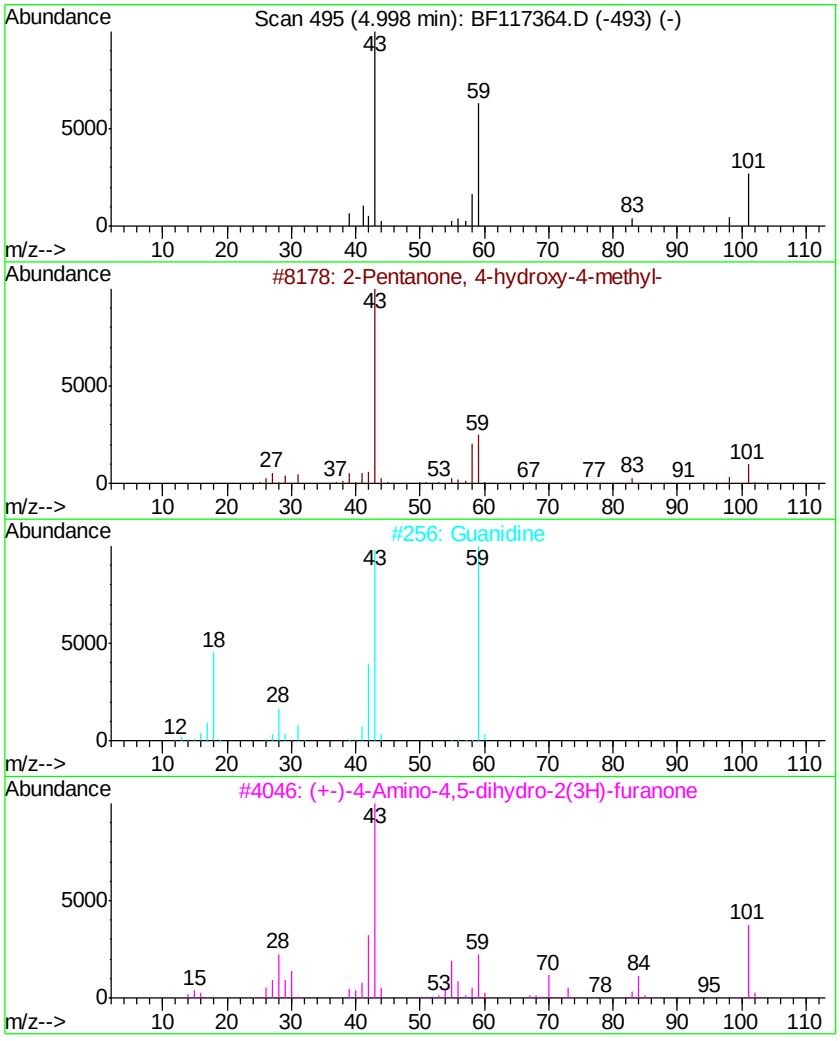
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

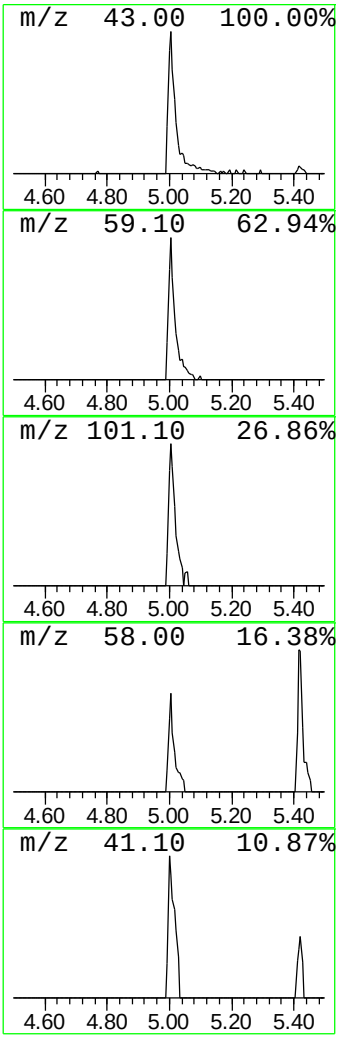
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.57 ng	55330	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Guanidine	59	CH5N3	000113-00-8	38
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





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Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

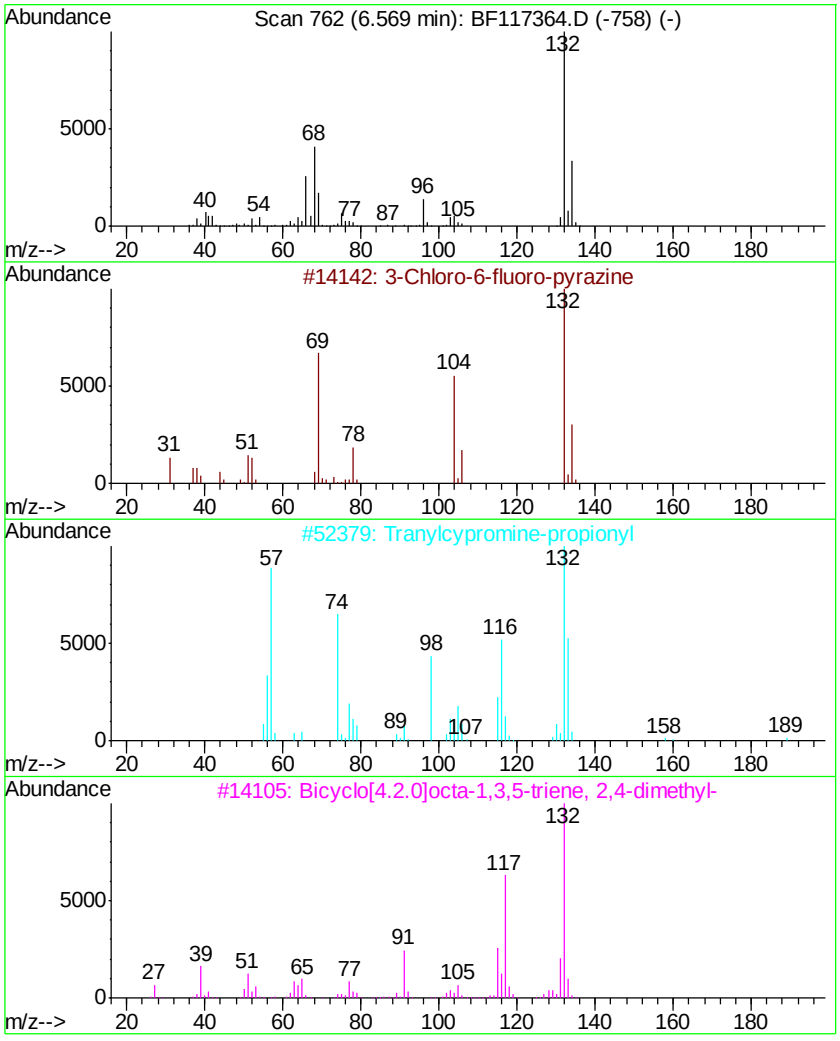
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

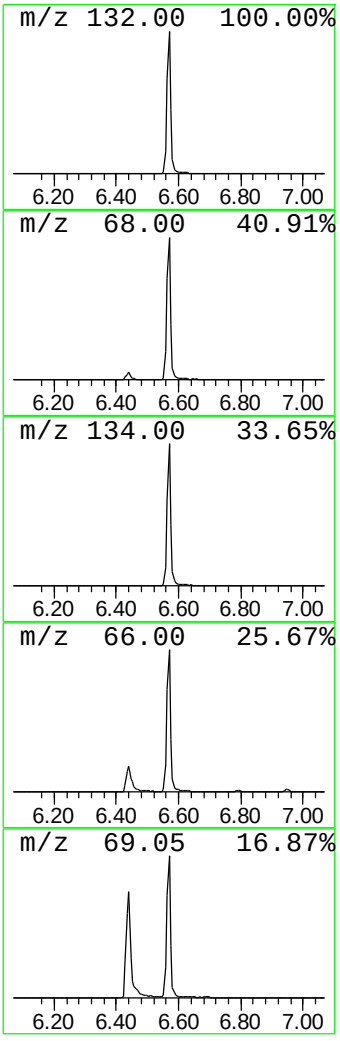
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	78.94 ng	956329	1,4-Dichlorobenzene-d4	6.79

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	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Acq On : 10 Oct 2019 17:08
Operator : JU
Sample : K5297-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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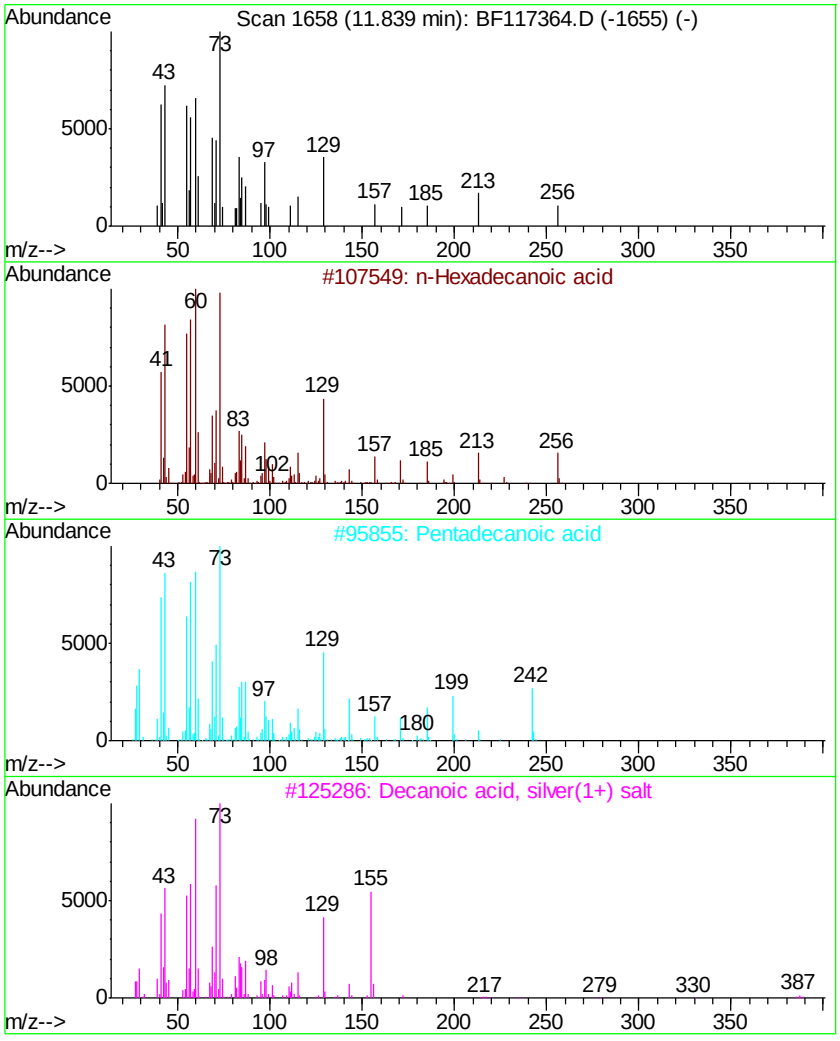
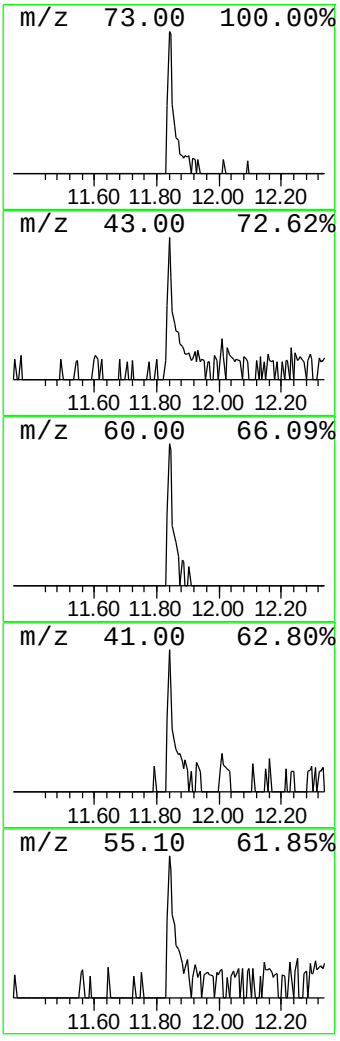
Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.28 ng	42459	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43





Library Search Compound Report

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Operator : JU
Sample : K5297-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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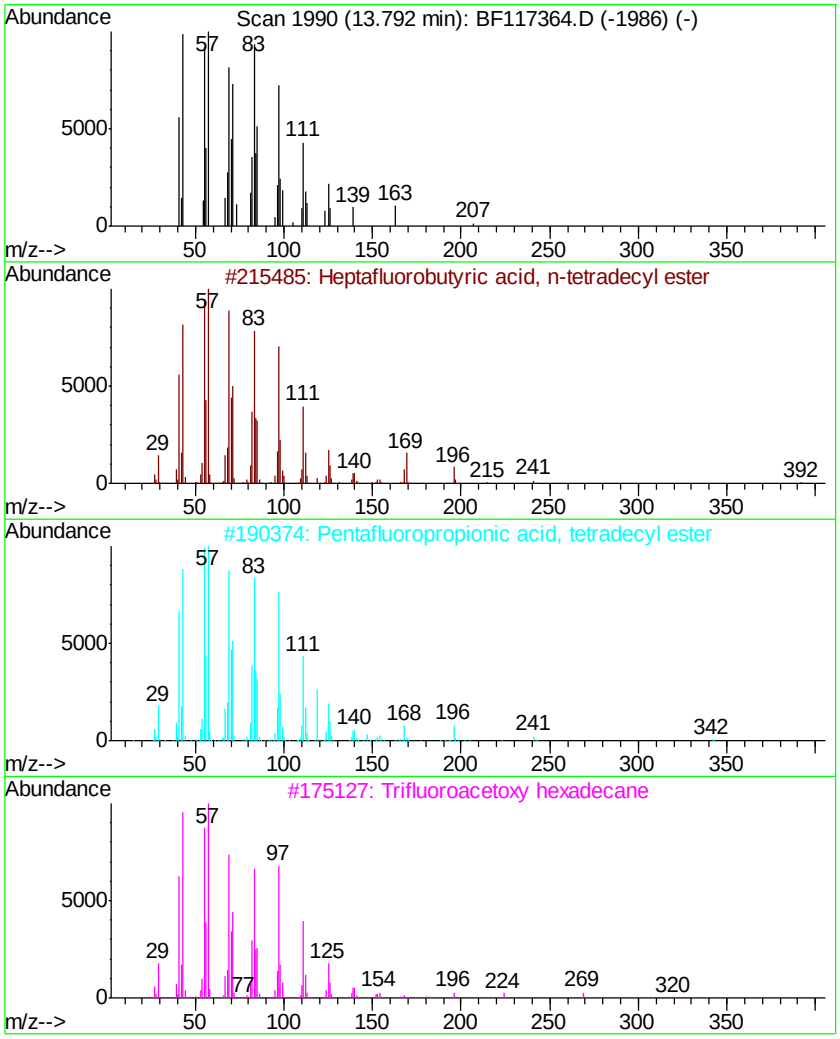
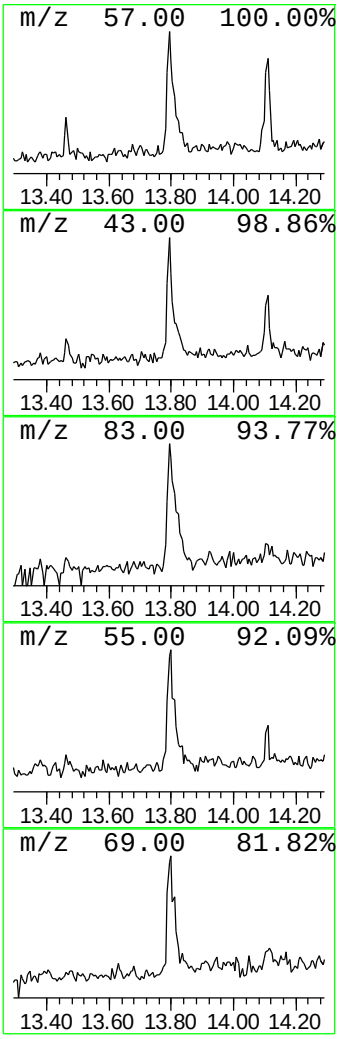
Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	5.74 ng	87850	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Behenic alcohol	326	C22H46O	000661-19-8	87
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





Library Search Compound Report

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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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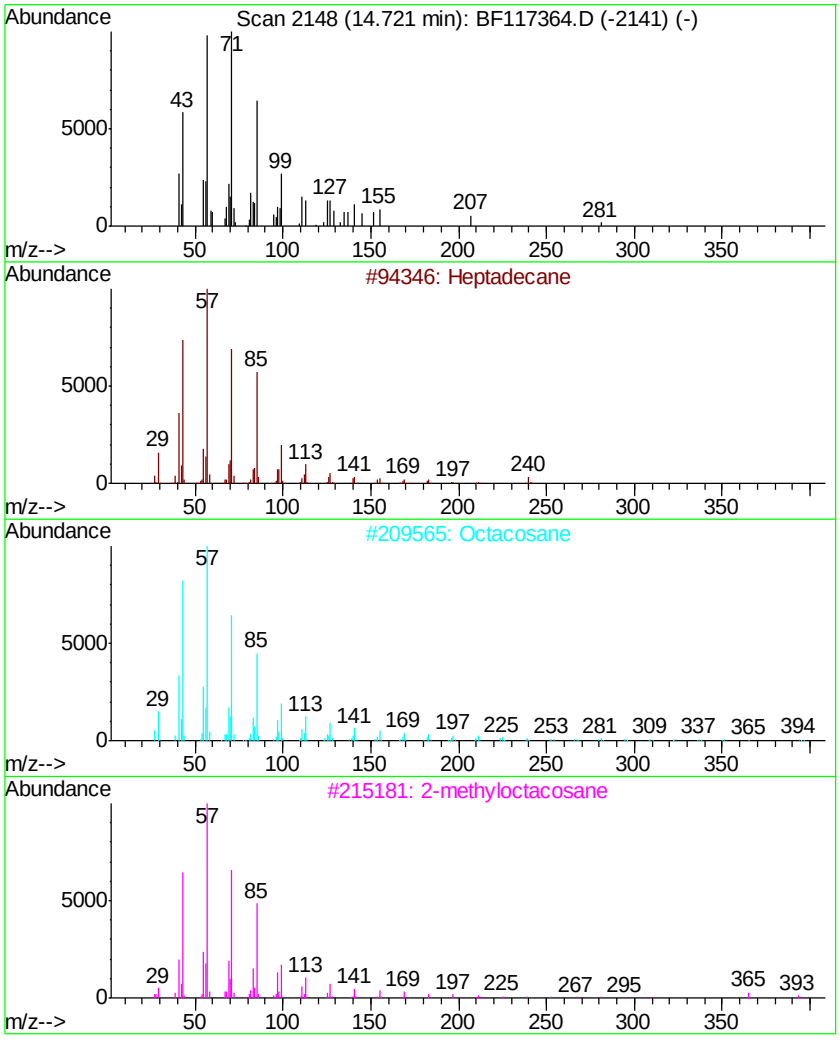
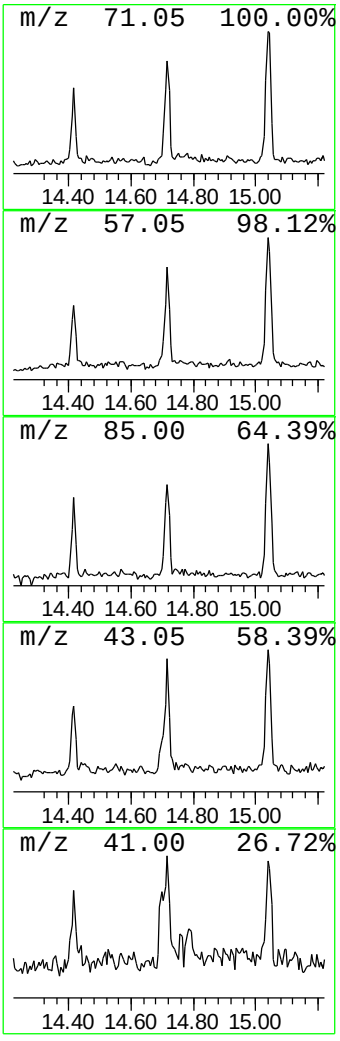
Peak Number 6 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	4.62 ng	72694	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Octacosane	394	C28H58	000630-02-4	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	10-Methylnonadecane	282	C20H42	056862-62-5	87
5	Heneicosane	296	C21H44	000629-94-7	87





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TIC Library : C:\DATABASE\NIST11.L
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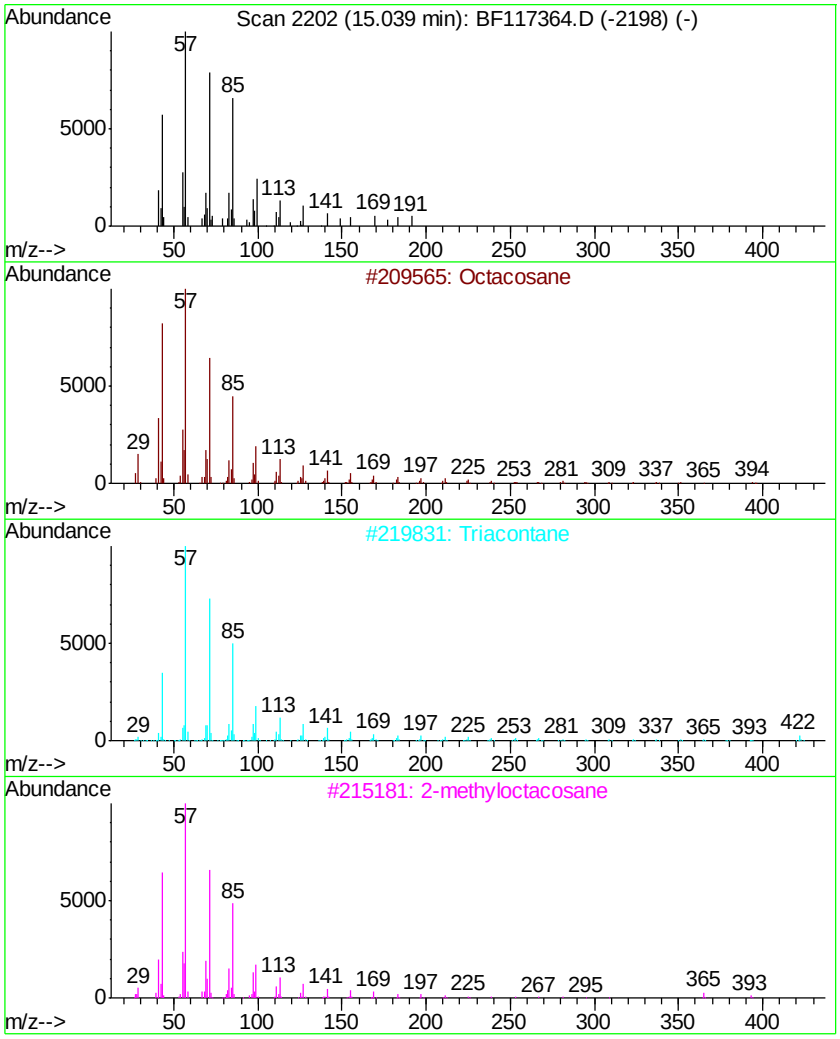
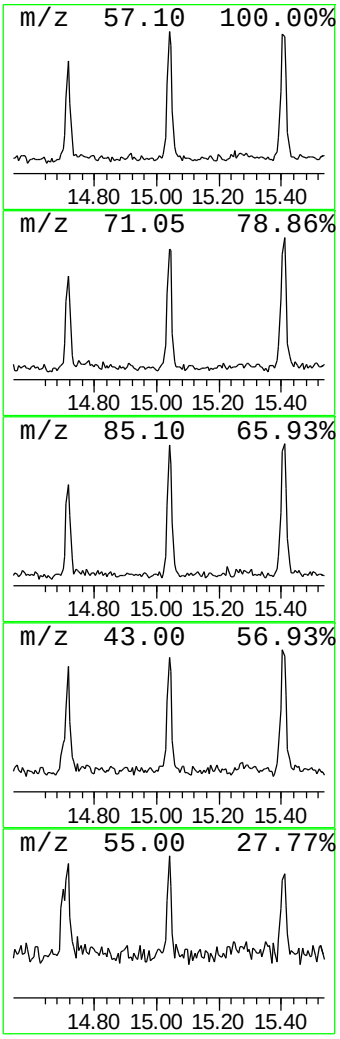
Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	5.02 ng	78972	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Triacontane	422	C30H62	000638-68-6	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane	296	C21H44	000629-94-7	83





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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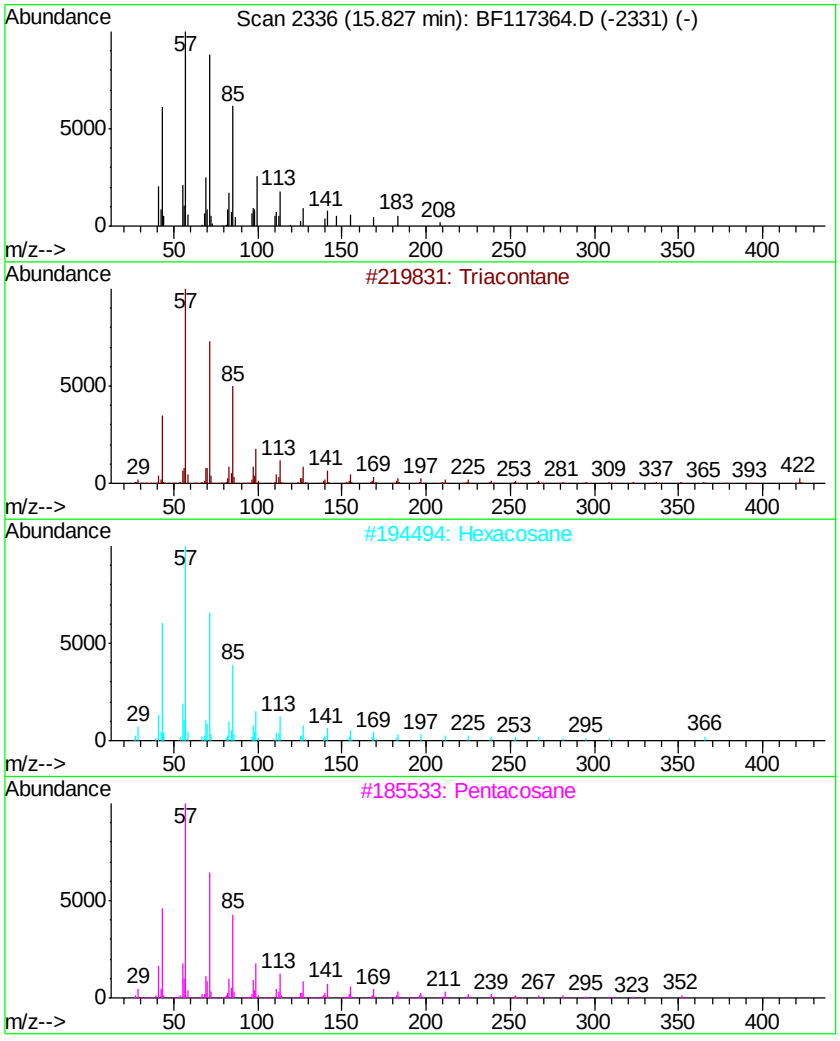
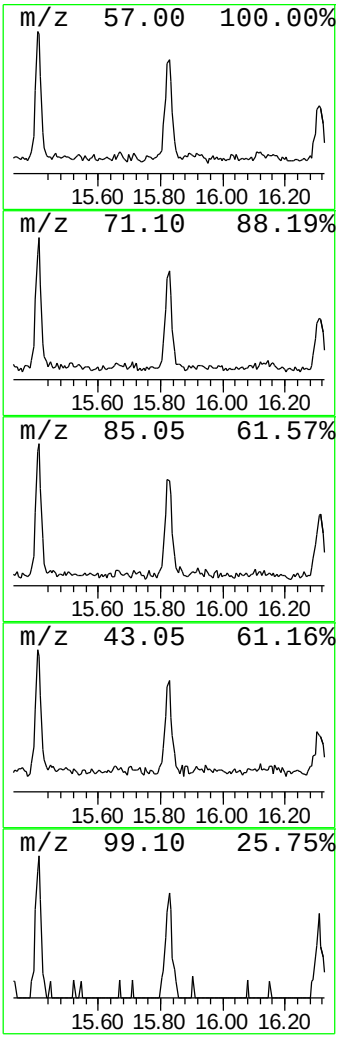
Peak Number 8 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	4.23 ng	66608	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	Heptadecane	240	C17H36	000629-78-7	78
5	Octadecane	254	C18H38	000593-45-3	78





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

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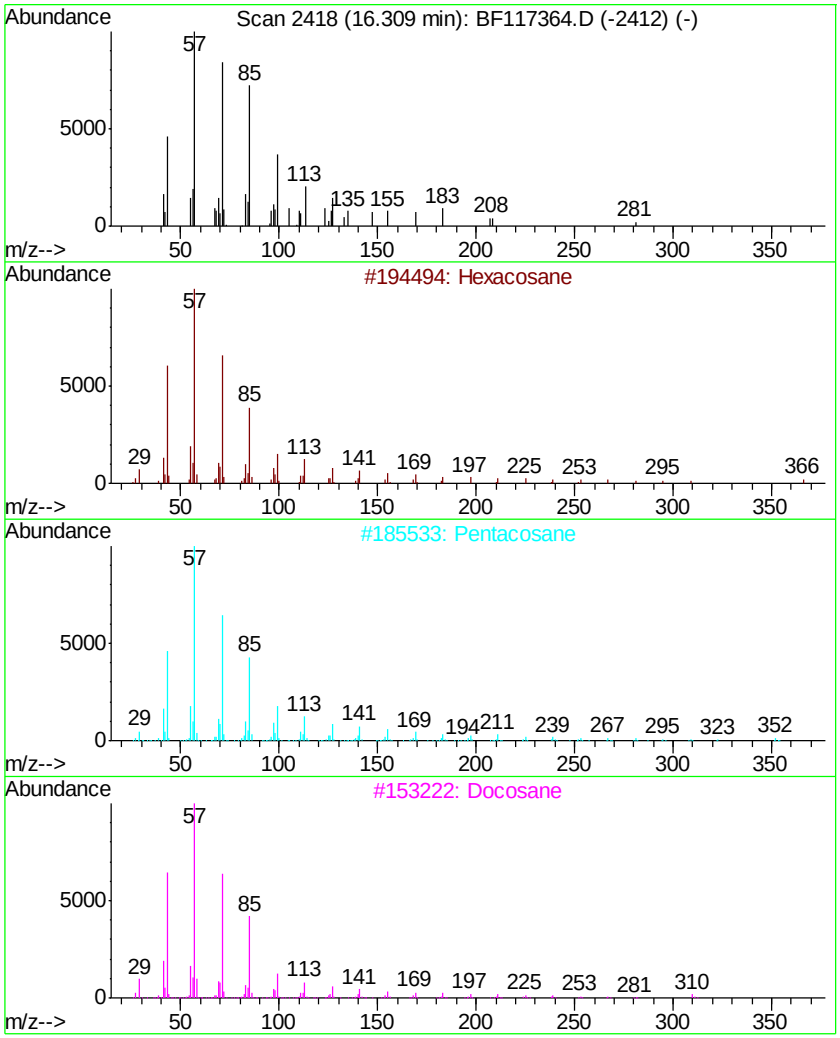
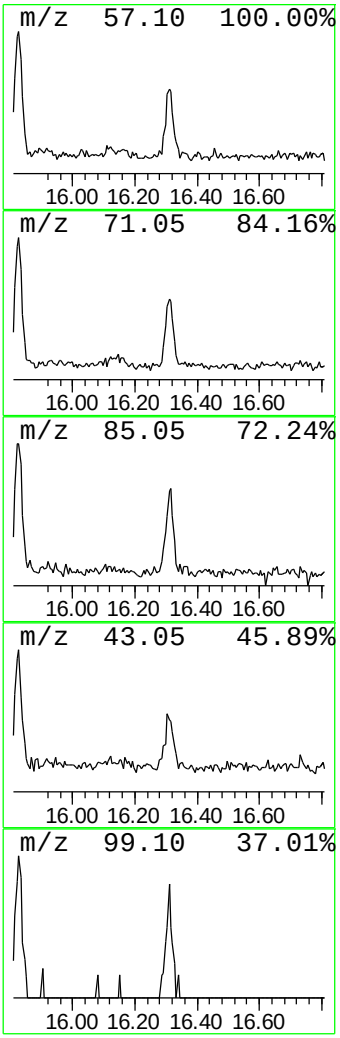
Peak Number 9 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	2.84 ng	44671	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Pentacosane	352	C25H52	000629-99-2	83
3	Docosane	310	C22H46	000629-97-0	78
4	Eicosane	282	C20H42	000112-95-8	78
5	Hentriacontane	437	C31H64	000630-04-6	72





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...	5.00	4.6	ng	55330	1	6.79	242306	20.0
unknown6.57	6.57	78.9	ng	956329	1	6.79	242306	20.0
n-Hexadecanoic acid	11.84	2.3	ng	42459	4	11.32	371981	20.0
Heptafluorobutyri...	13.79	5.7	ng	87850	5	13.96	306065	20.0
Heptadecane	14.72	4.6	ng	72694	6	15.42	314942	20.0
Octacosane	15.04	5.0	ng	78972	6	15.42	314942	20.0
Triacontane	15.83	4.2	ng	66608	6	15.42	314942	20.0
Hexacosane	16.31	2.8	ng	44671	6	15.42	314942	20.0