LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082218\
Data File : BF108400.D
Acq On : 22 Aug 2018 23:00
Operator : JU/SJ
Sample : J4572-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F-1

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-BF080818.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	2.390	3	9	22	rVB	693715	979738	17.38%	2.230%
2	5.272	495	499	509	rVB	143182	223307	3.96%	0.508%
3	5.637	555	561	564	rBV	4246008	4769579	84.62%	10.857%
4	6.631	723	730	733	rBV	4111448	5250785	93.16%	11.952%
5	6.778	749	755	758	rBV	4774086	5001792	88.74%	11.385%
6	7.001	789	793	797	rBV	1205402	949487	16.85%	2.161%
7	7.160	815	820	823	rBV	4155142	3678707	65.27%	8.374%
8	7.566	883	889	892	rBV	2847892	3254864	57.75%	7.409%
9	8.283	1007	1011	1015	rBV	1352862	1132639	20.09%	2.578%
10	9.360	1188	1194	1197	rBV	5763696	5636434	100.00%	12.830%
11	9.748	1256	1260	1263	rBV	753275	574763	10.20%	1.308%
12	10.048	1307	1311	1315	rBV	1440876	1238727	21.98%	2.820%
13	10.842	1441	1446	1449	rBV	3268103	3008361	53.37%	6.848%
14	11.542	1561	1565	1569	rBV	1322191	1115871	19.80%	2.540%
15	13.130	1830	1835	1838	rBV	4611370	4406420	78.18%	10.030%
16	13.677	1924	1928	1930	rBV2	97117	82307	1.46%	0.187%
17	14.007	1981	1984	1988	rVB	102111	83264	1.48%	0.190%
18	14.071	1990	1995	2004	rBV4	44878	120091	2.13%	0.273%
19	14.195	2012	2016	2021	rBV	943016	838368	14.87%	1.908%
20	14.324	2034	2038	2041	rBV	124909	110379	1.96%	0.251%
21	14.630	2087	2090	2094	rBV	123429	121827	2.16%	0.277%
22	14.954	2140	2145	2150	rBV3	126793	175906	3.12%	0.400%
23	15.318	2203	2207	2214	rVB	102117	123923	2.20%	0.282%
24	15.748	2273	2280	2288	rVB	566930	869970	15.43%	1.980%
25	16.206	2354	2358	2364	rVB	77411	116658	2.07%	0.266%
26	16.759	2448	2452	2458	rBV	39563	68384	1.21%	0.156%

Sum of corrected areas: 43932551

LSC Report - Integrated Chromatogram

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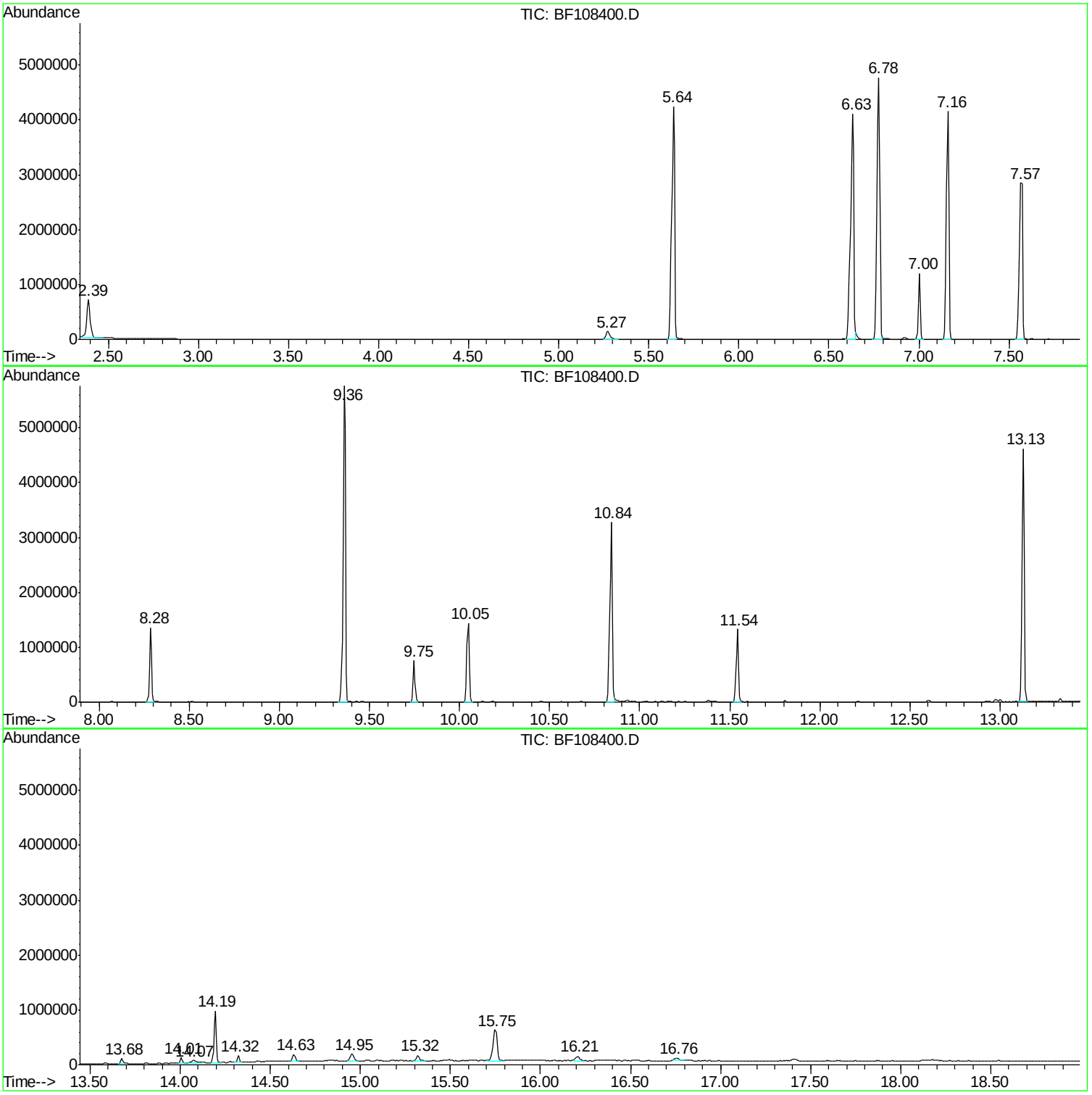
Sample : J4572-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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 : BF108400.D
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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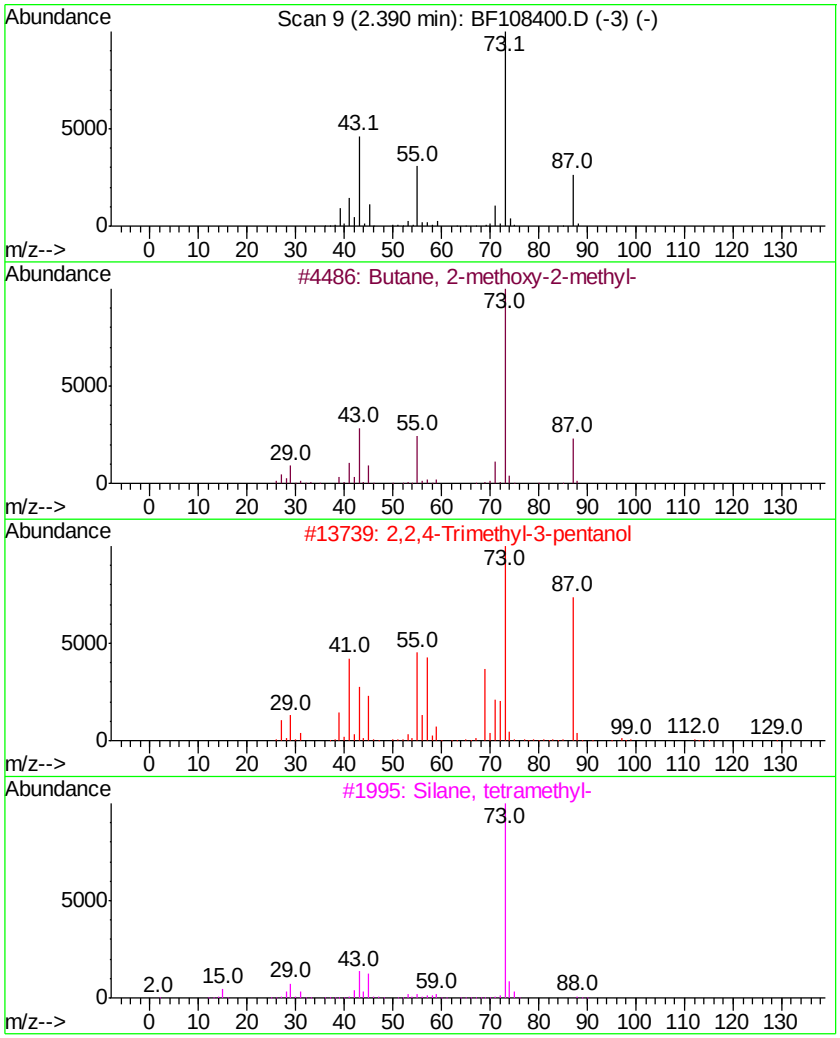
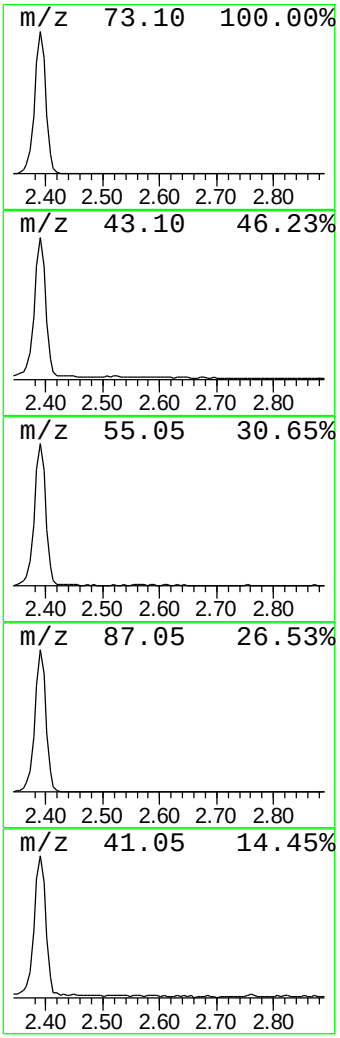
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.39	20.64 ng	979738	1,4-Dichlorobenzene-d4	7.00

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Sample : J4572-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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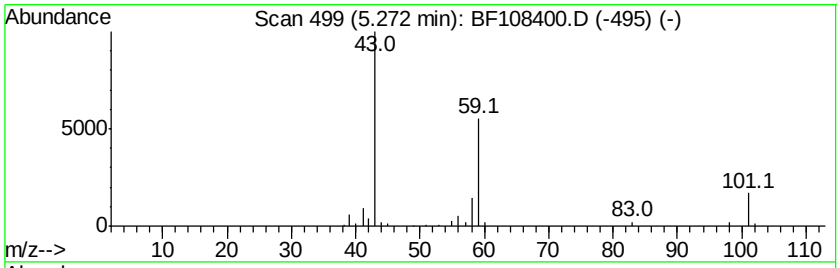
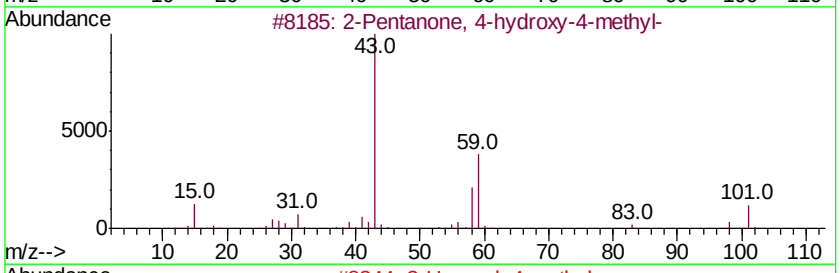
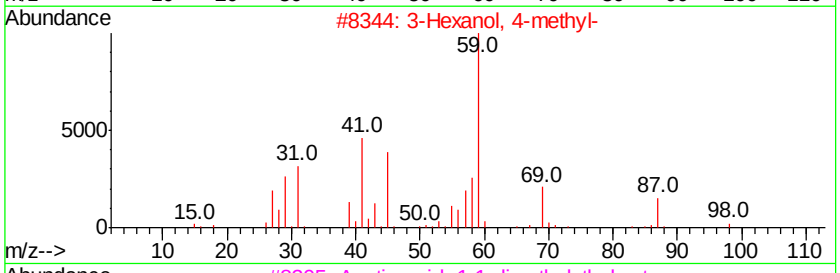
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

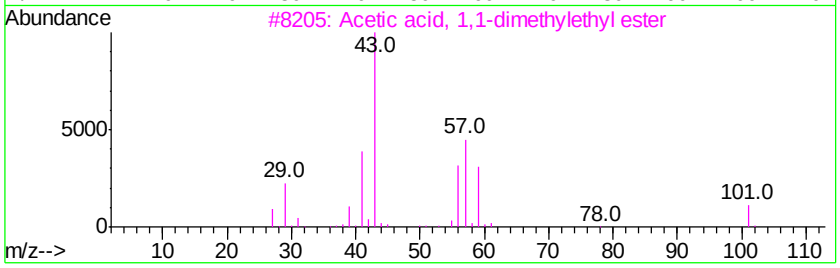
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	4.70 ng	223307	1,4-Dichlorobenzene-d4	7.00

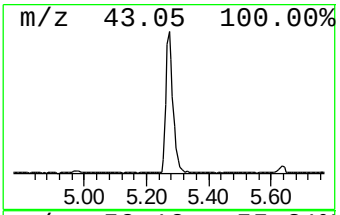
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

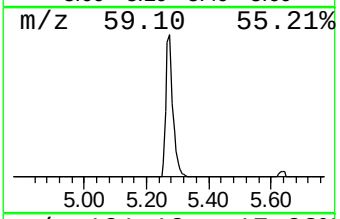


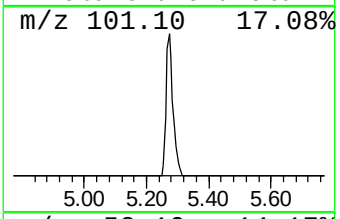


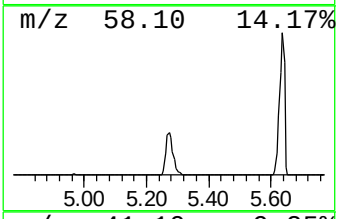


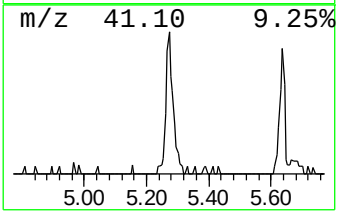












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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

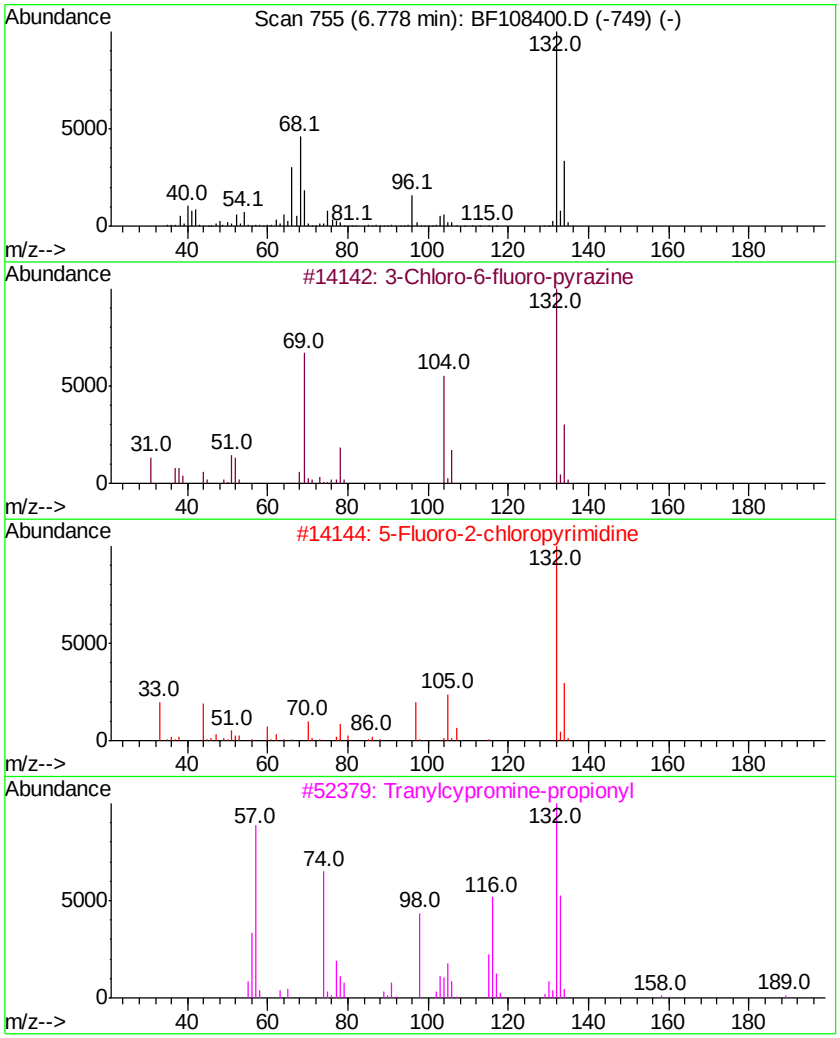
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

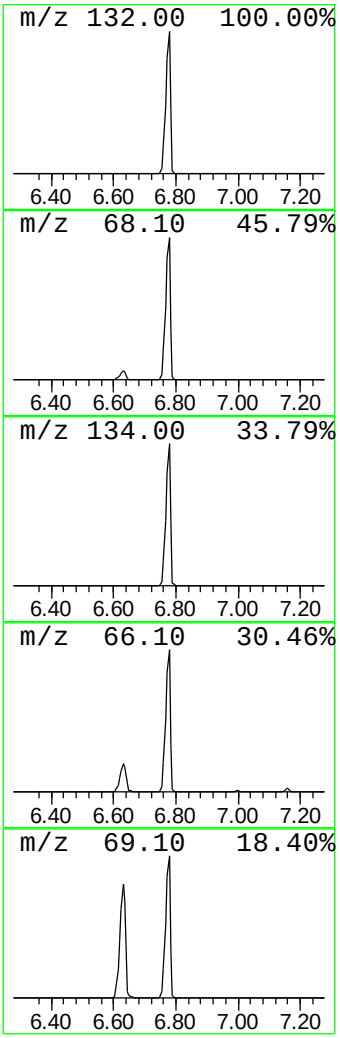
****

Peak Number 3 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	105.36 ng	5001790	1,4-Dichlorobenzene-d4	7.00

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

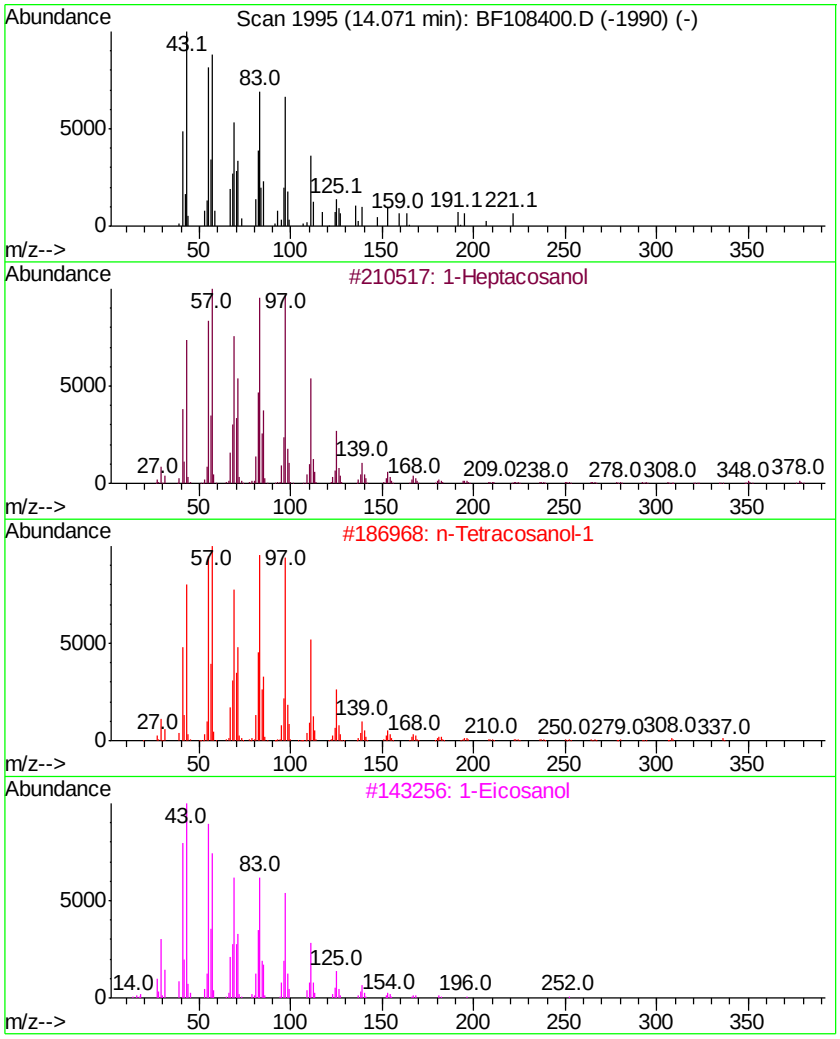
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

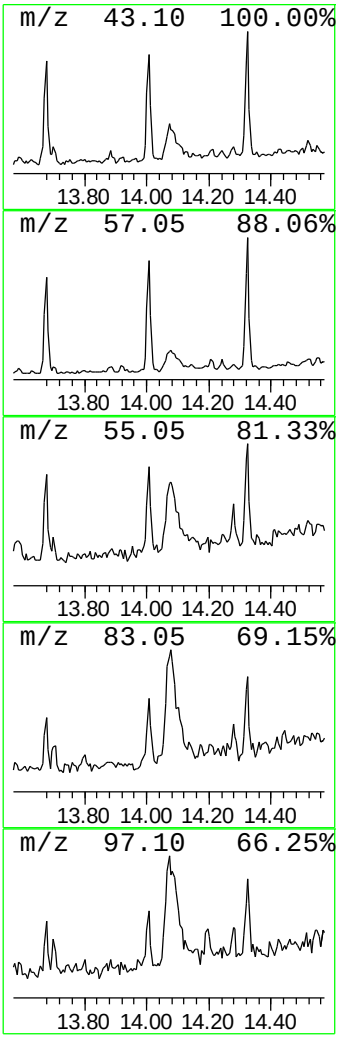
****

Peak Number 5 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.86 ng	120091	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	87
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	1-Eicosanol	298	C20H42O	000629-96-9	87
4	Behenic alcohol	326	C22H46O	000661-19-8	87
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





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Instrument : BNA_F
ClientSampleId : F-1

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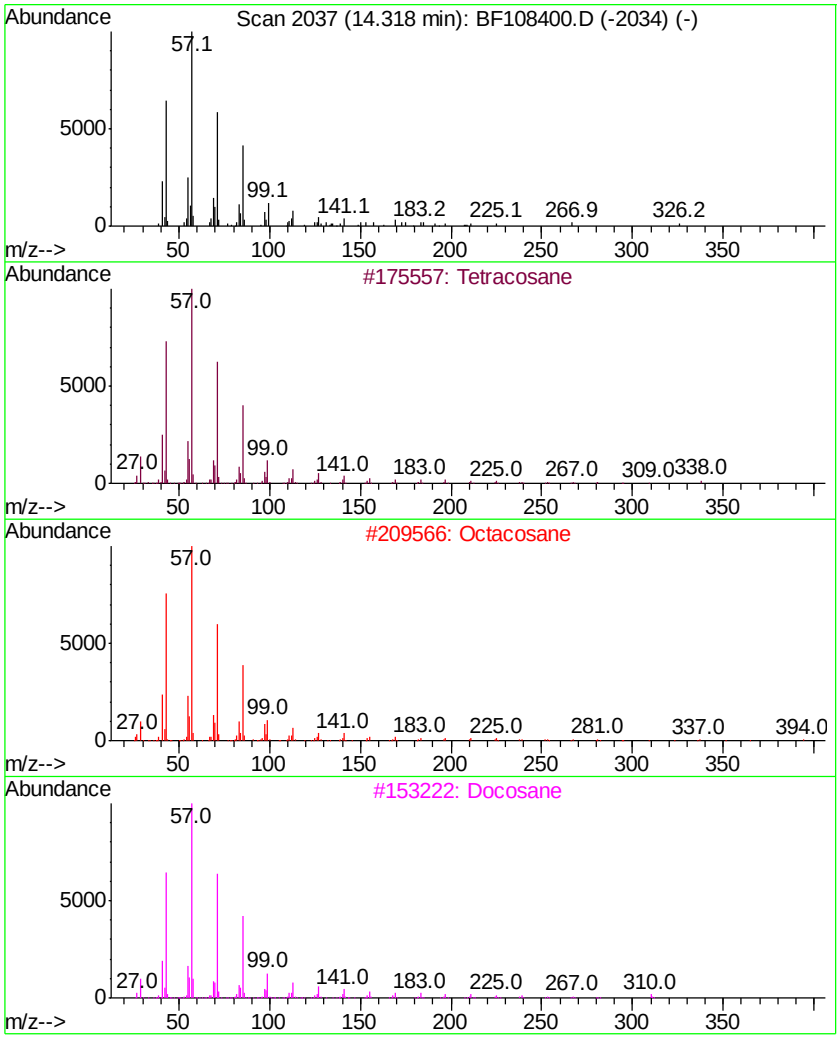
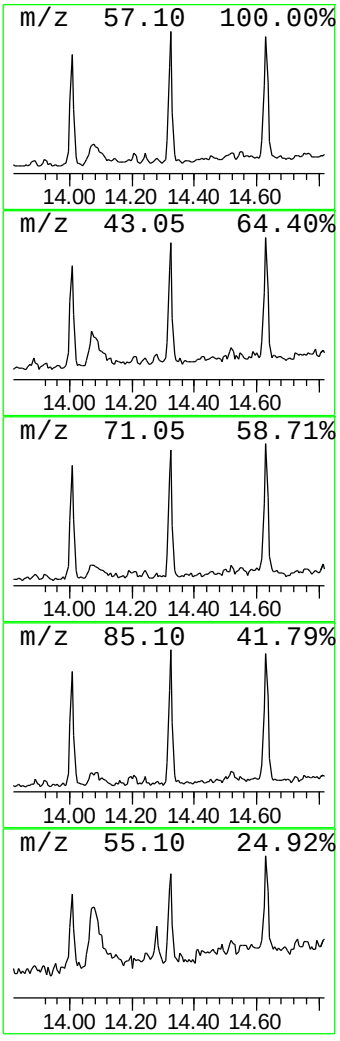
Peak Number 6 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.63 ng	110379	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Docosane	310	C22H46	000629-97-0	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Hexacosane	366	C26H54	000630-01-3	90





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : F-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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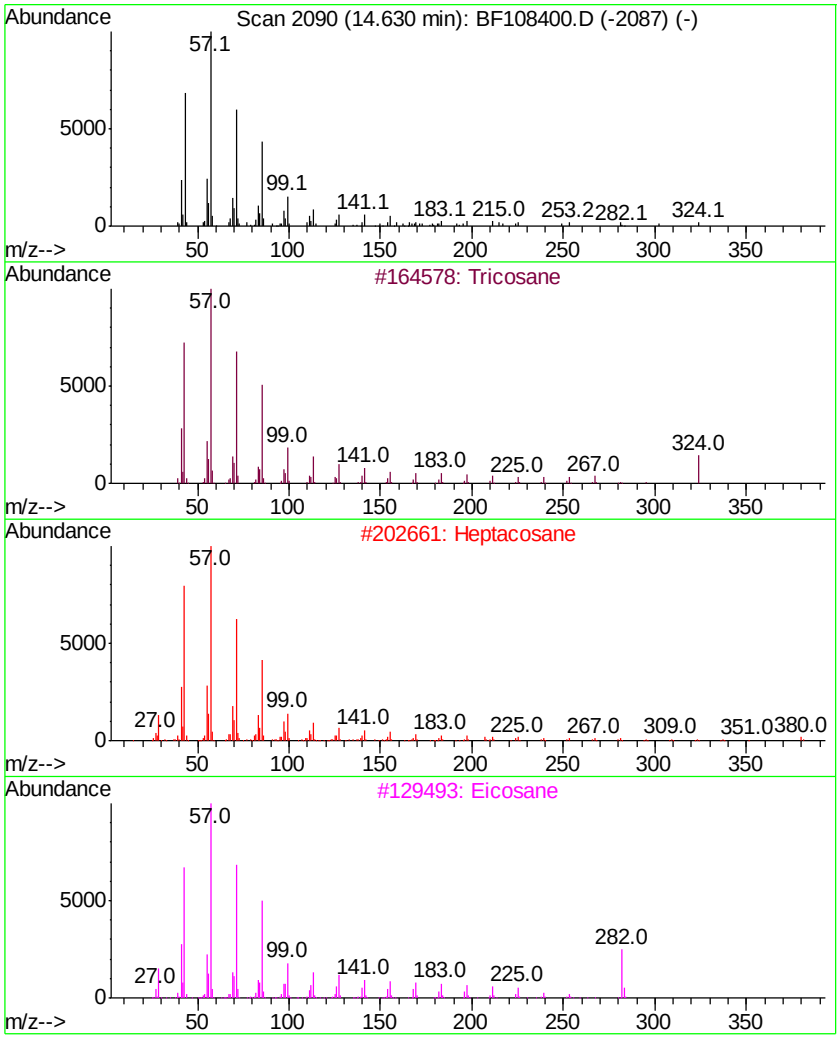
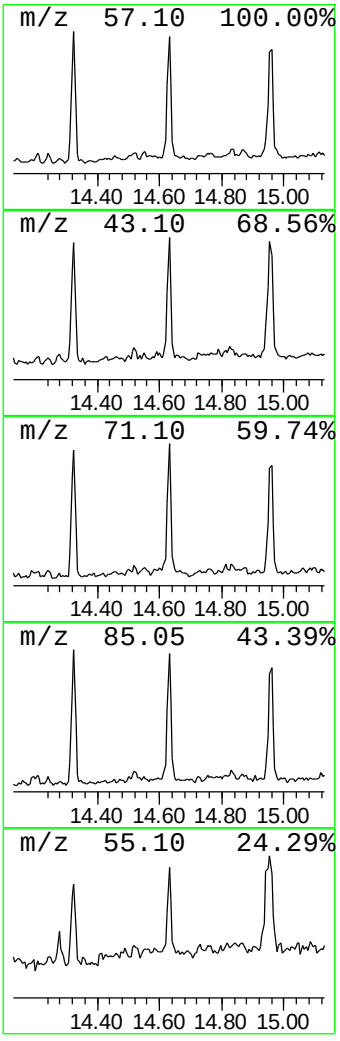
Peak Number 7 Tricosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.91 ng	121827	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Heptacosane	380	C27H56	000593-49-7	90
3	Eicosane	282	C20H42	000112-95-8	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Hentriacontane	437	C31H64	000630-04-6	87





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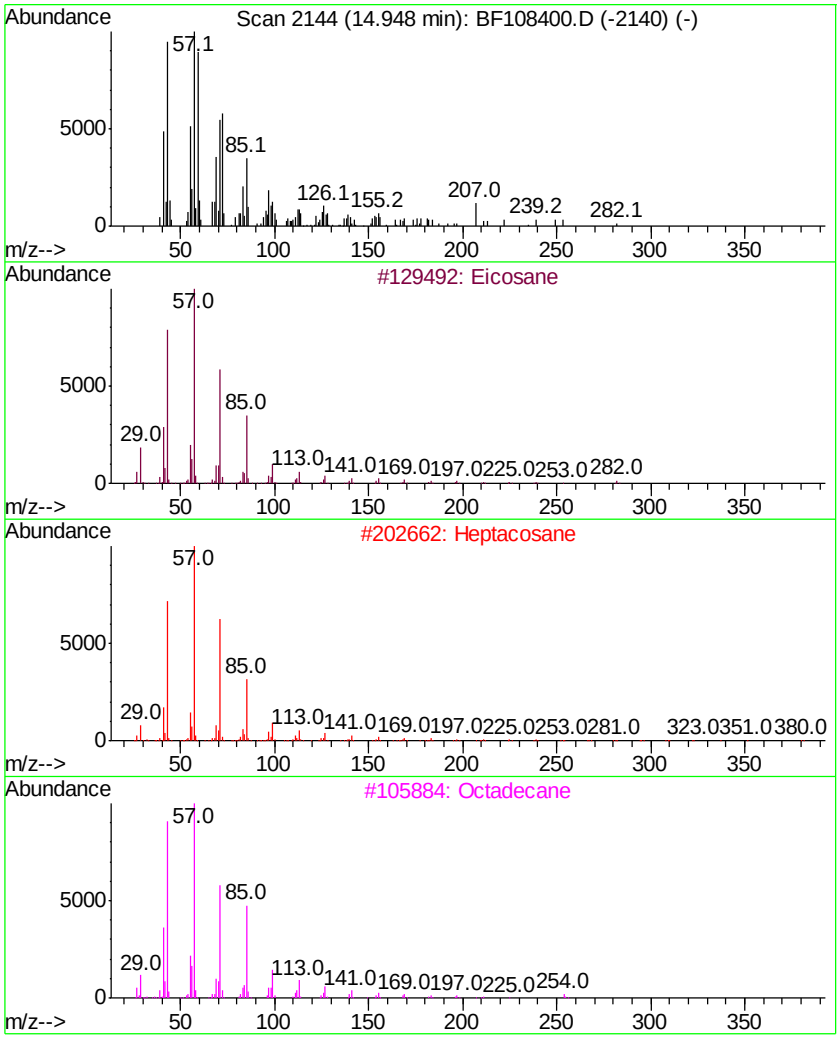
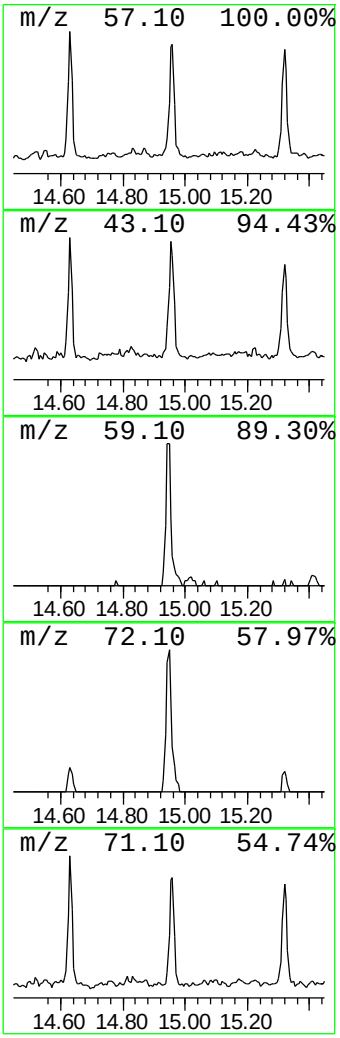
Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	4.20 ng	175906	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	68
2	Heptacosane	380	C27H56	000593-49-7	64
3	Octadecane	254	C18H38	000593-45-3	64
4	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	64
5	Heptadecane	240	C17H36	000629-78-7	64





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

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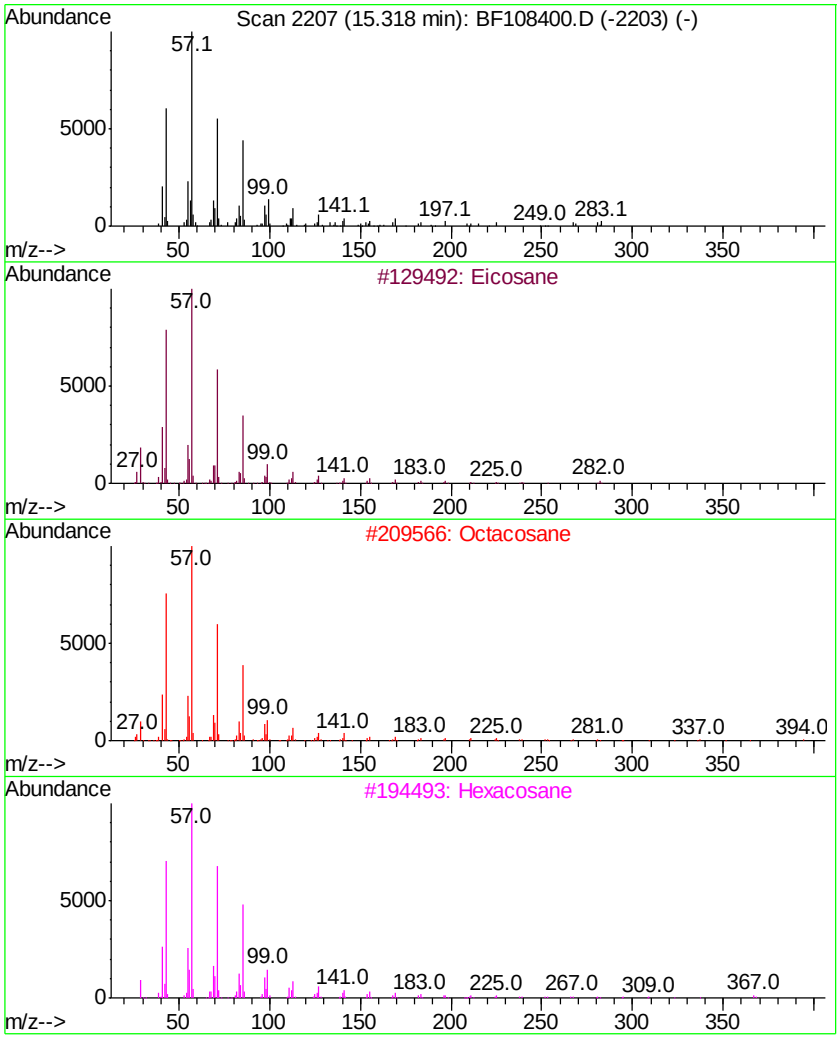
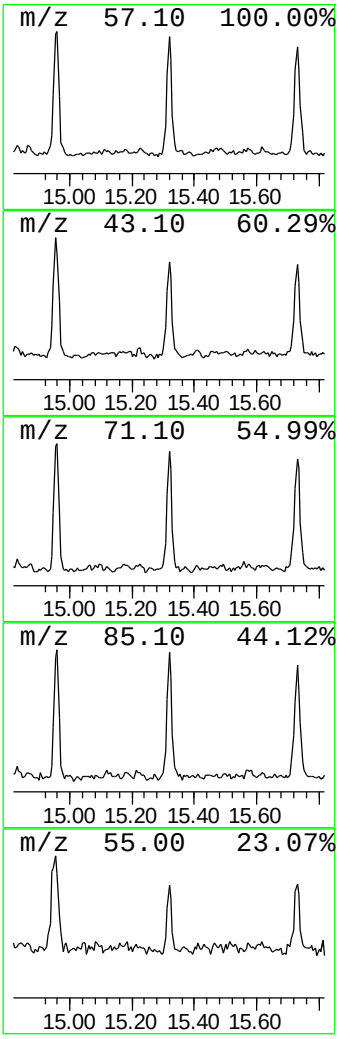
Peak Number 9 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	2.85 ng	123923	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Tetracosane	338	C24H50	000646-31-1	91





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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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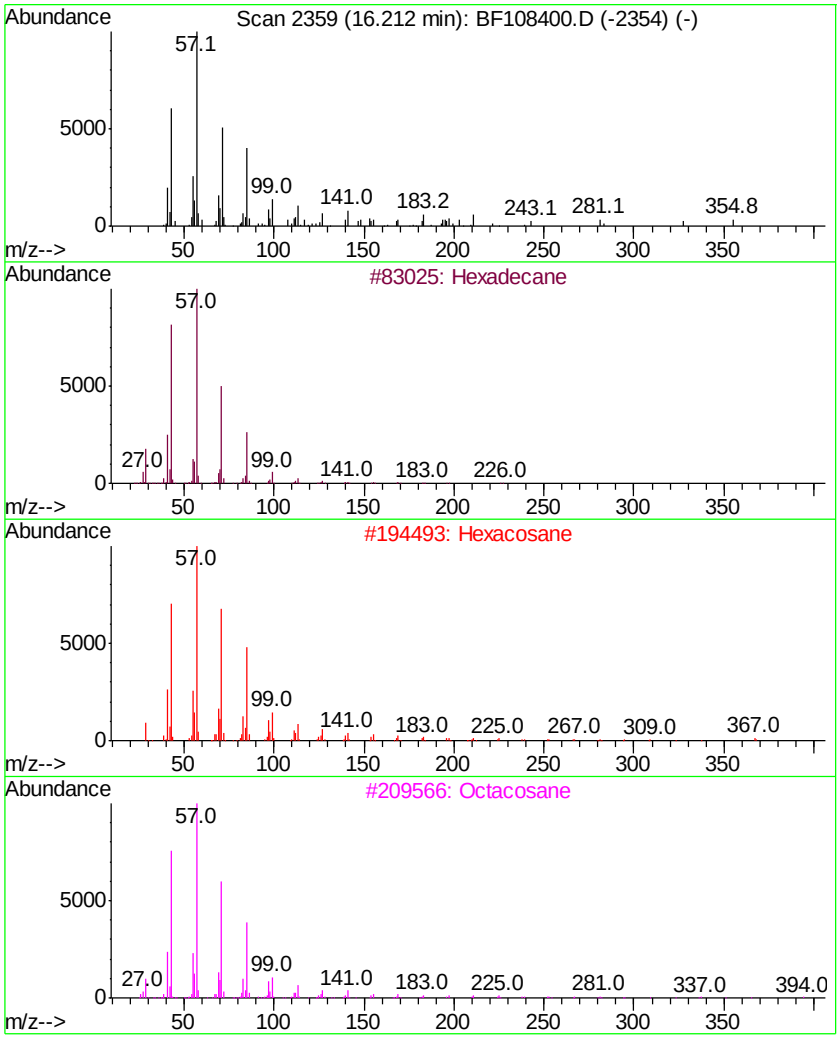
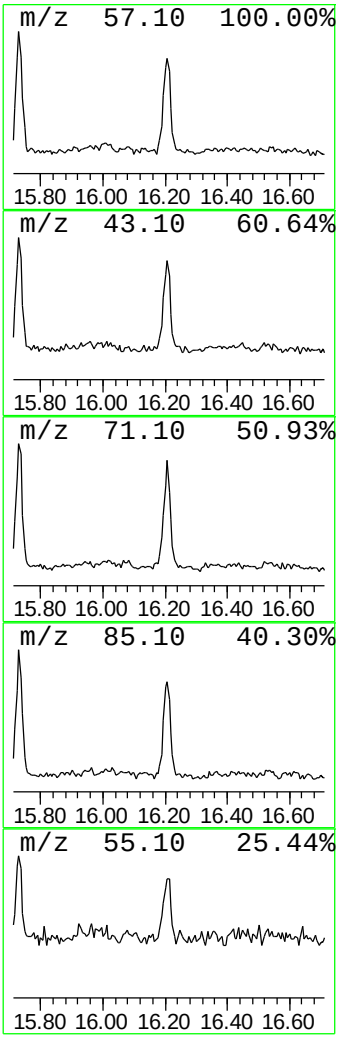
Peak Number 10 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.68 ng	116658	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Hexacosane	366	C26H54	000630-01-3	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Pentacosane	352	C25H52	000629-99-2	86
5	Hexatriacontane	507	C36H74	000630-06-8	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082218\
Data File : BF108400.D
Acq On : 22 Aug 2018 23:00
Operator : JU/SJ
Sample : J4572-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	2.39	20.6	ng	979738	1	7.00	949487	20.0
2-Pentanone, 4-hy...	5.27	4.7	ng	223307	1	7.00	949487	20.0
unknown6.78	6.78	105.4	ng	5001790	1	7.00	949487	20.0
1-Heptacosanol	14.07	2.9	ng	120091	5	14.19	838368	20.0
Tetracosane	14.32	2.6	ng	110379	5	14.19	838368	20.0
Tricosane	14.63	2.9	ng	121827	5	14.19	838368	20.0
Eicosane	14.95	4.2	ng	175906	5	14.19	838368	20.0
Hexacosane	15.32	2.9	ng	123923	6	15.75	869970	20.0
Hexadecane	16.21	2.7	ng	116658	6	15.75	869970	20.0