LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099425.D
Acq On : 13 Oct 2017 6:58
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.134	4	8	31	rVB	174966	289025	9.64%	1.563%
2	5.069	504	507	519	rVB	156467	168657	5.62%	0.912%
3	5.475	572	576	590	rBV	971006	961791	32.08%	5.200%
4	6.481	744	747	765	rBV	729370	686948	22.91%	3.714%
5	6.622	767	771	774	rBV	1968945	1666892	55.59%	9.012%
6	6.851	807	810	814	rBV	780147	624547	20.83%	3.377%
7	7.010	832	837	840	rBV	2581348	2332842	77.80%	12.612%
8	7.422	901	907	910	rBV	1752842	1750651	58.38%	9.465%
9	8.133	1024	1028	1036	rBV	981131	809291	26.99%	4.375%
10	9.210	1205	1211	1214	rBV	3285043	2998510	100.00%	16.211%
11	9.886	1322	1326	1330	rBV	839353	728768	24.30%	3.940%
12	10.674	1457	1460	1475	rBV	832901	843628	28.13%	4.561%
13	11.374	1575	1579	1583	rBV	723579	617227	20.58%	3.337%
14	12.957	1844	1848	1852	rBV	2300564	2259825	75.36%	12.217%
15	14.015	2024	2028	2038	rBV	686703	612541	20.43%	3.312%
16	15.104	2208	2213	2220	rVB	42206	52796	1.76%	0.285%
17	15.486	2272	2278	2289	rBV2	374523	536987	17.91%	2.903%
18	15.909	2345	2350	2356	rBV	87062	121826	4.06%	0.659%
19	16.409	2430	2435	2444	rBV	83207	143257	4.78%	0.774%
20	16.998	2529	2535	2541	rBV	57955	118098	3.94%	0.638%
21	17.692	2647	2653	2663	rVB3	44079	104118	3.47%	0.563%
22	18.515	2788	2793	2805	rVB5	23103	68582	2.29%	0.371%

Sum of corrected areas: 18496807

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
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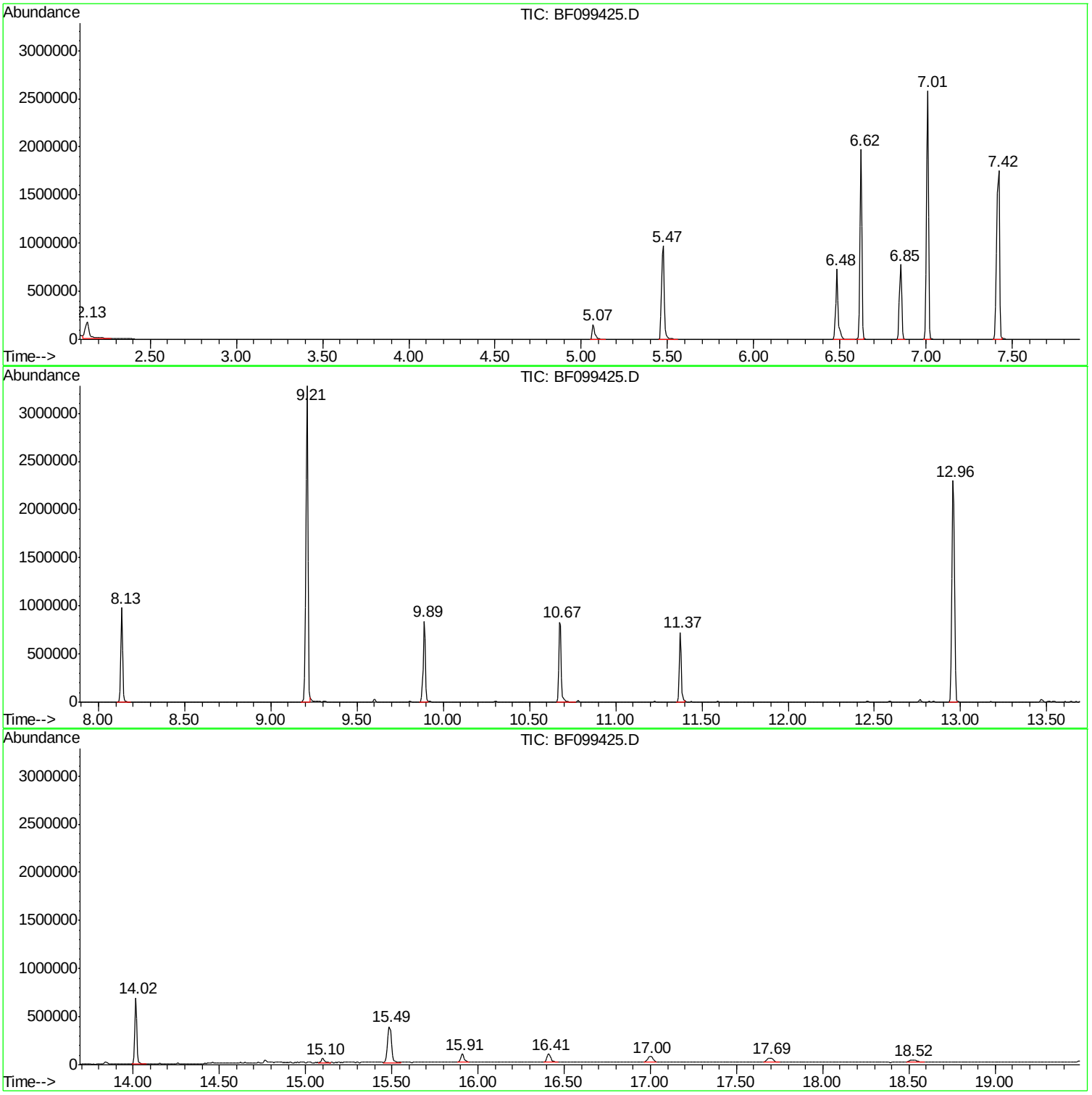
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099425.D
Acq On : 13 Oct 2017 6:58
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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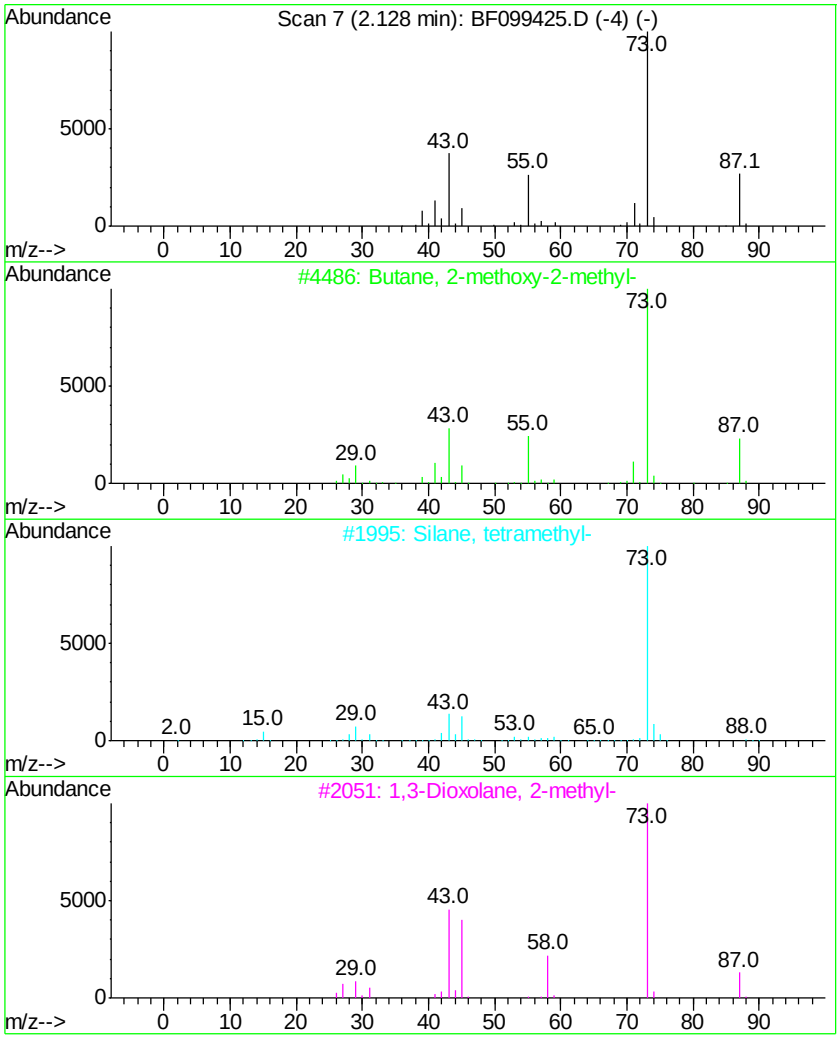
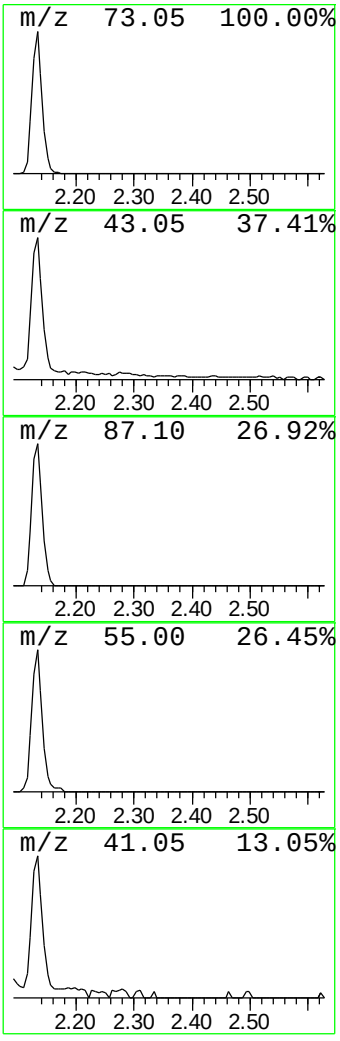
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	9.26 ng	289025	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099425.D
Acq On : 13 Oct 2017 6:58
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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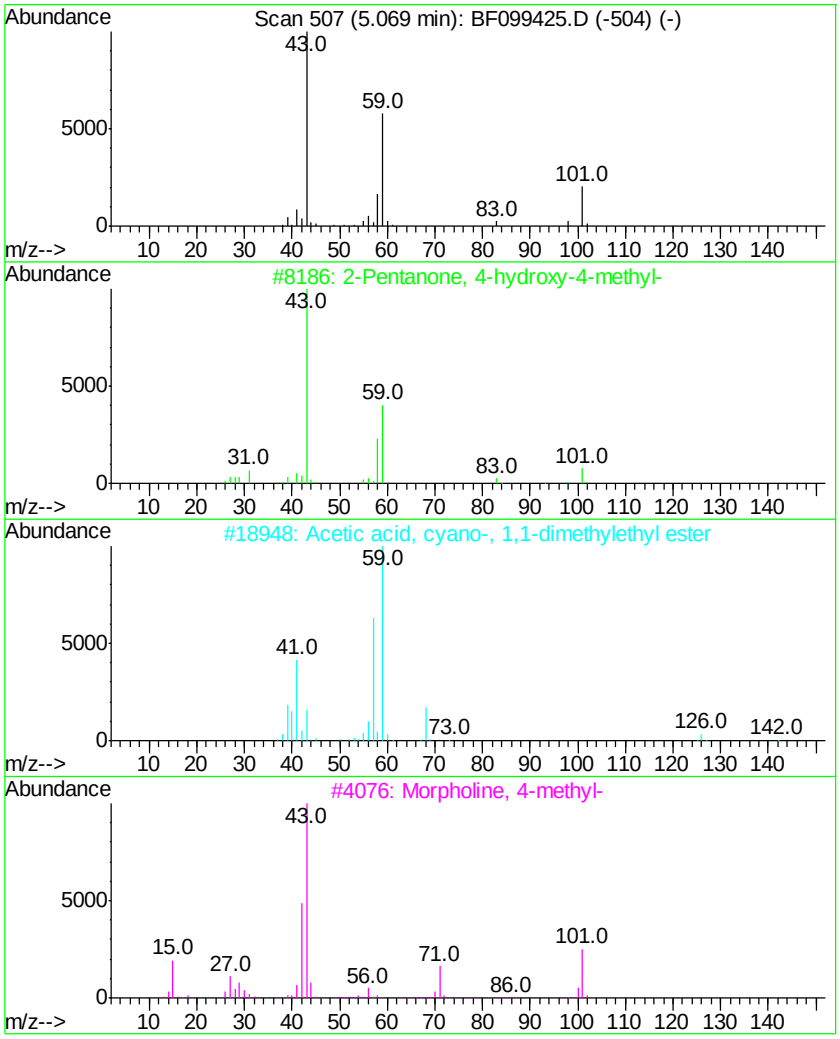
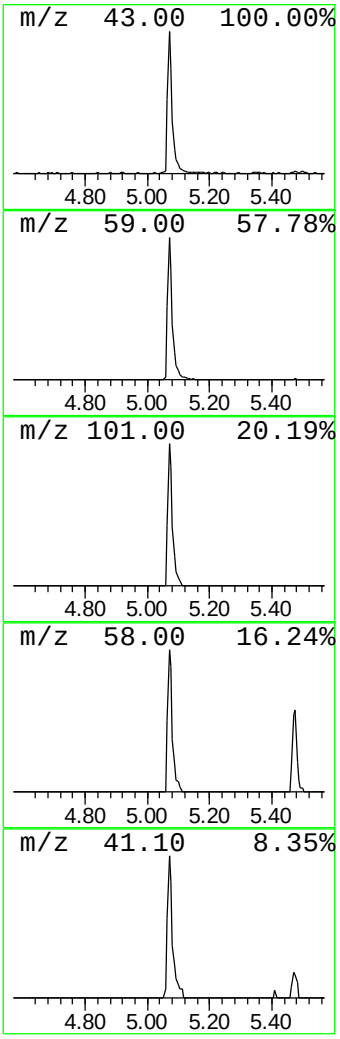
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	5.40 ng	168657	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





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Data File : BF099425.D
Acq On : 13 Oct 2017 6:58
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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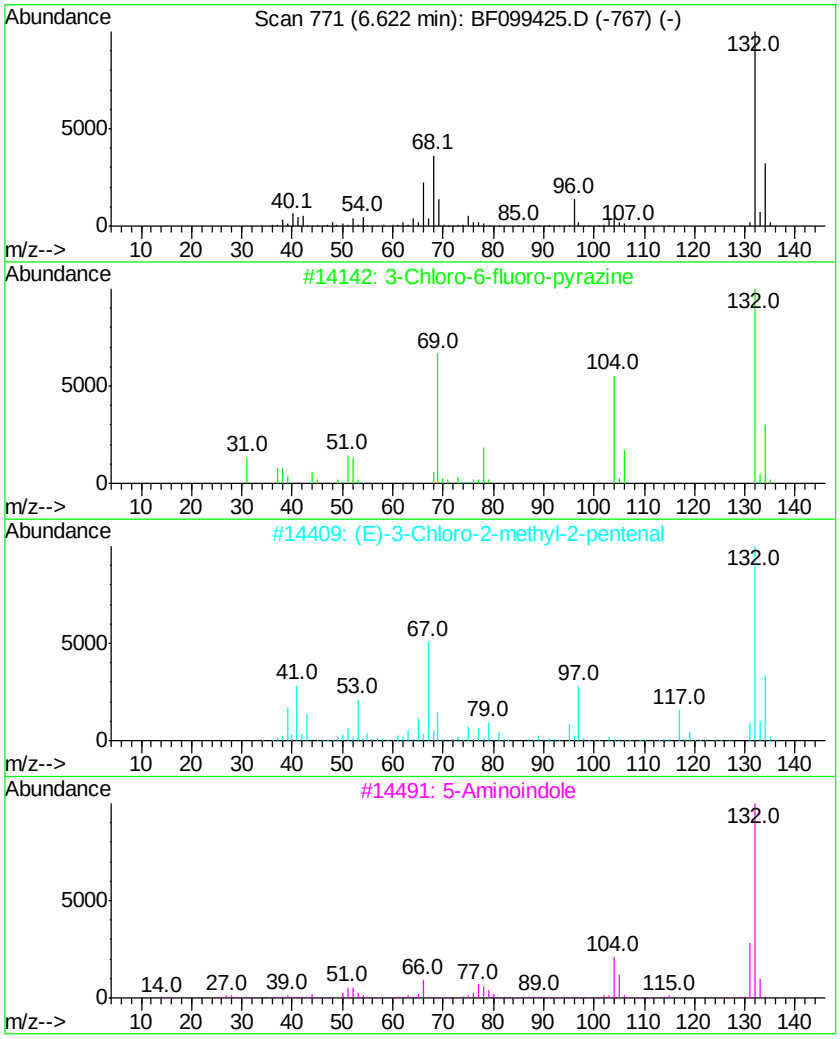
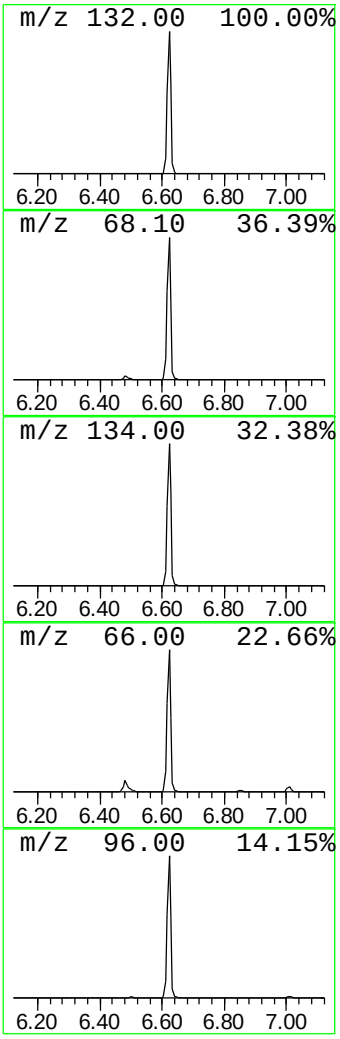
Peak Number 3 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	53.38 ng	1666890	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Data File : BF099425.D
Acq On : 13 Oct 2017 6:58
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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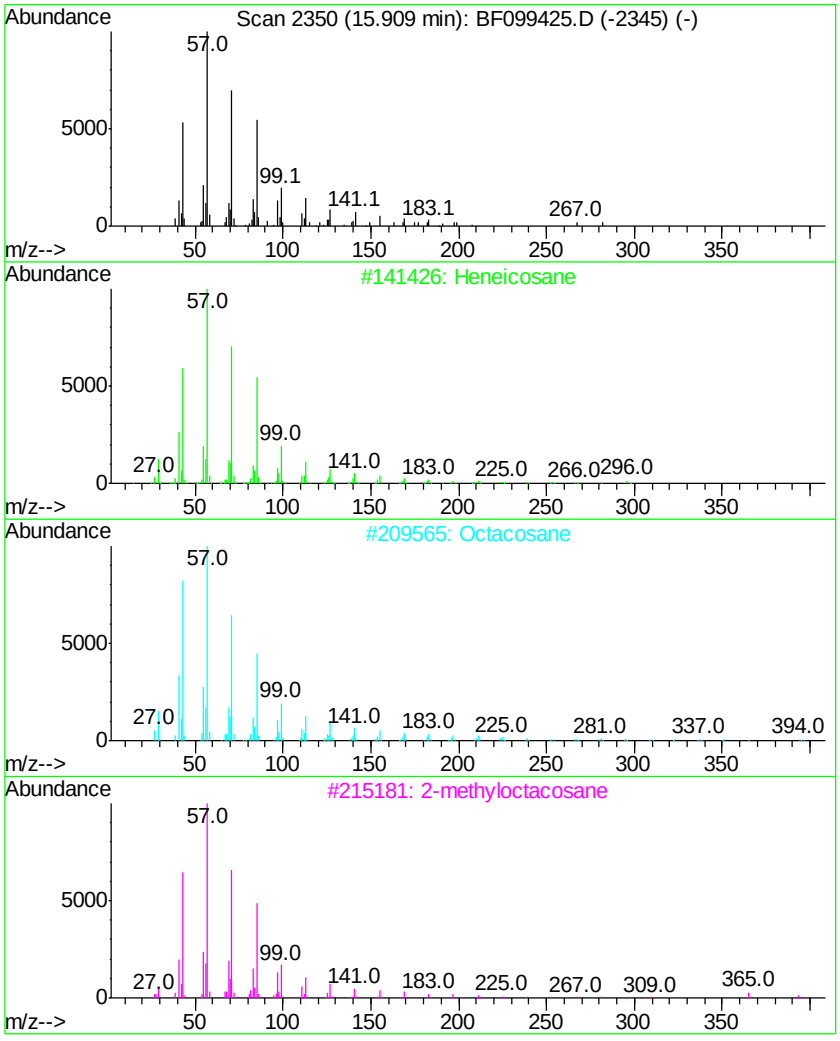
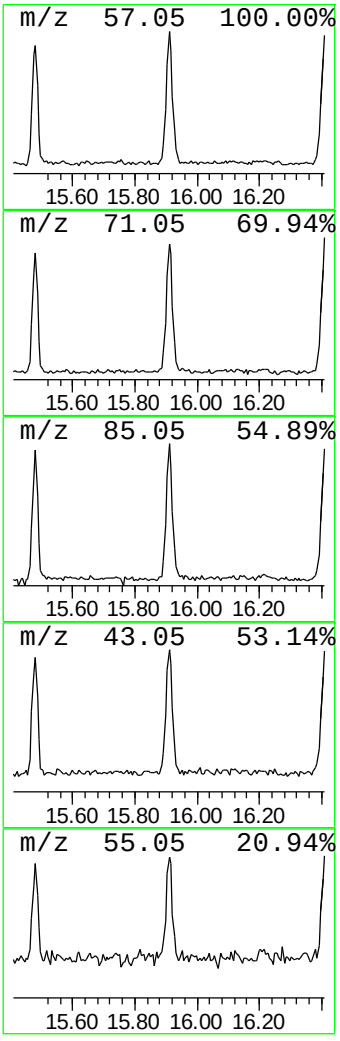
Peak Number 5 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	4.54 ng	121826	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Hexacosane	366	C26H54	000630-01-3	87





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Data File : BF099425.D
Acq On : 13 Oct 2017 6:58
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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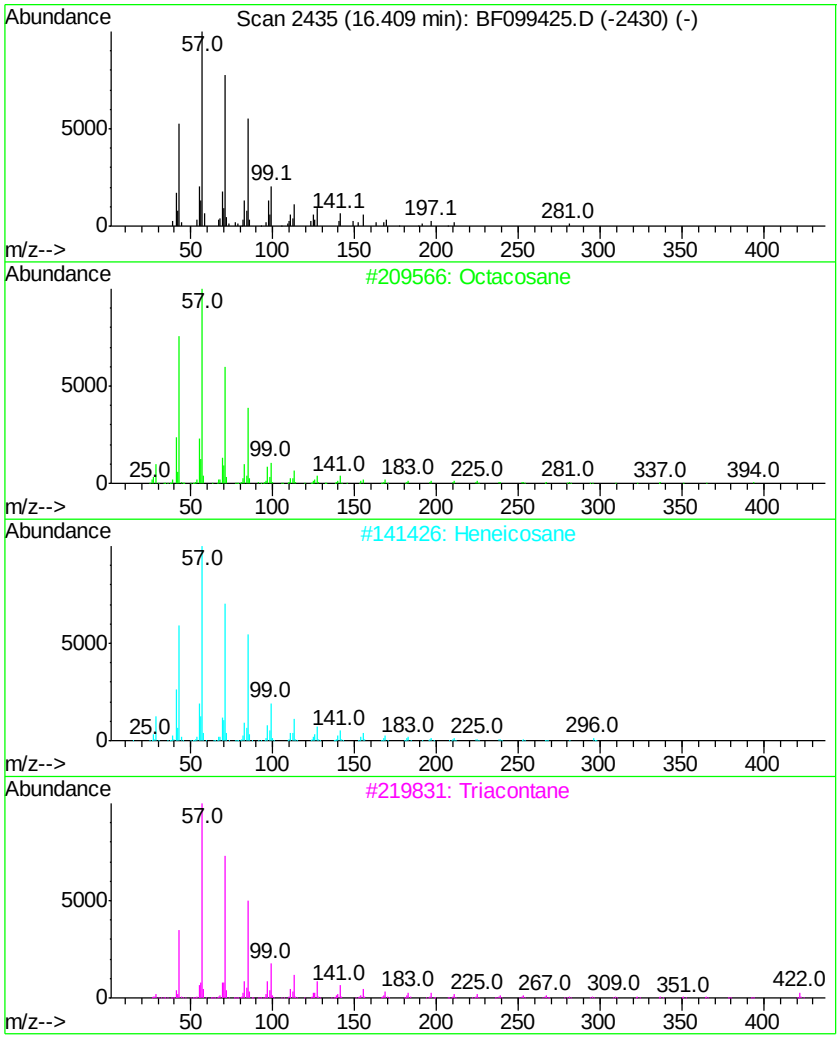
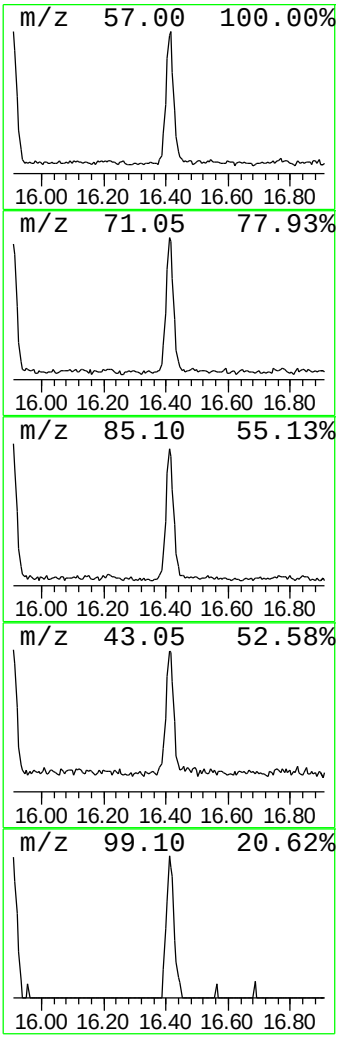
Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	5.34 ng	143257	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Triacontane	422	C30H62	000638-68-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Pentacosane	352	C25H52	000629-99-2	91





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Data File : BF099425.D
Acq On : 13 Oct 2017 6:58
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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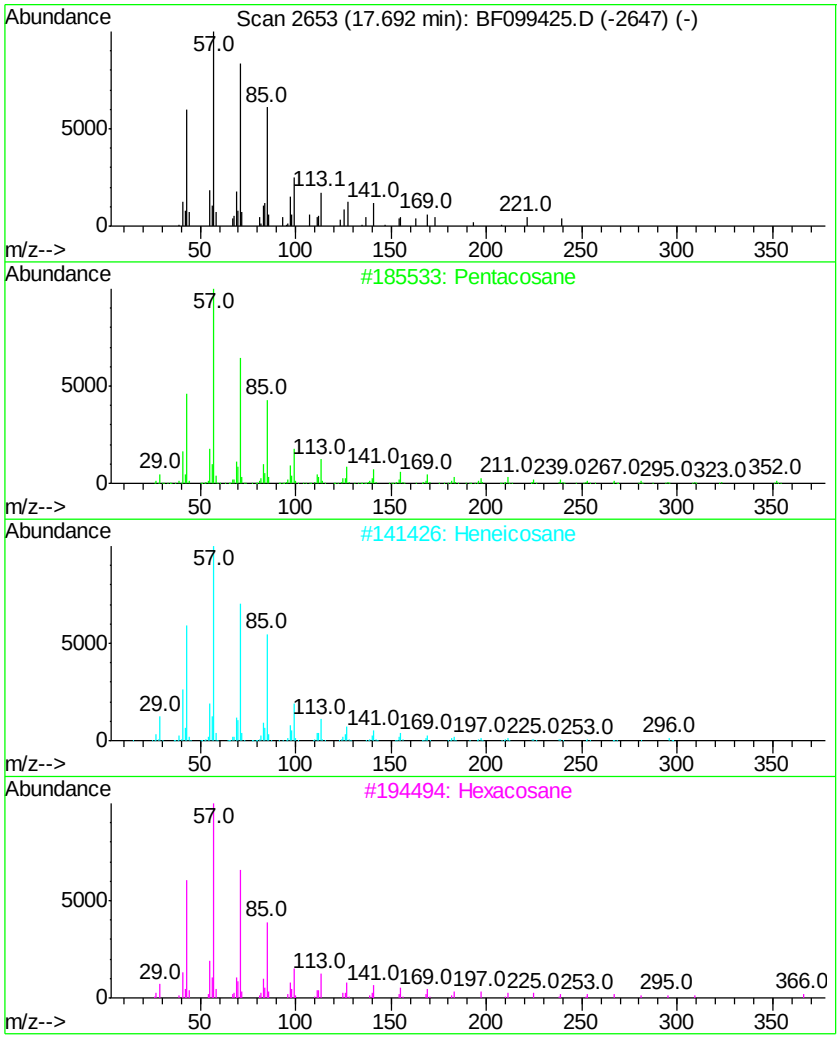
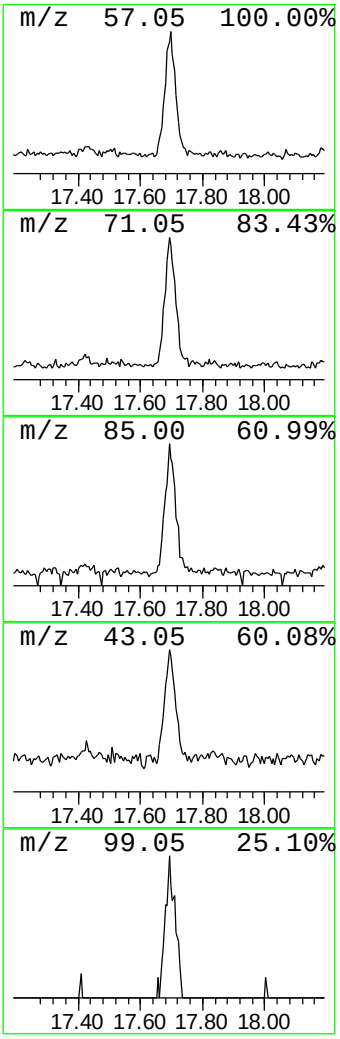
Peak Number 8 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.69	3.88 ng	104118	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	86
4	Tetratriacontane	479	C34H70	014167-59-0	83
5	Hentriacontane	437	C31H64	000630-04-6	80





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Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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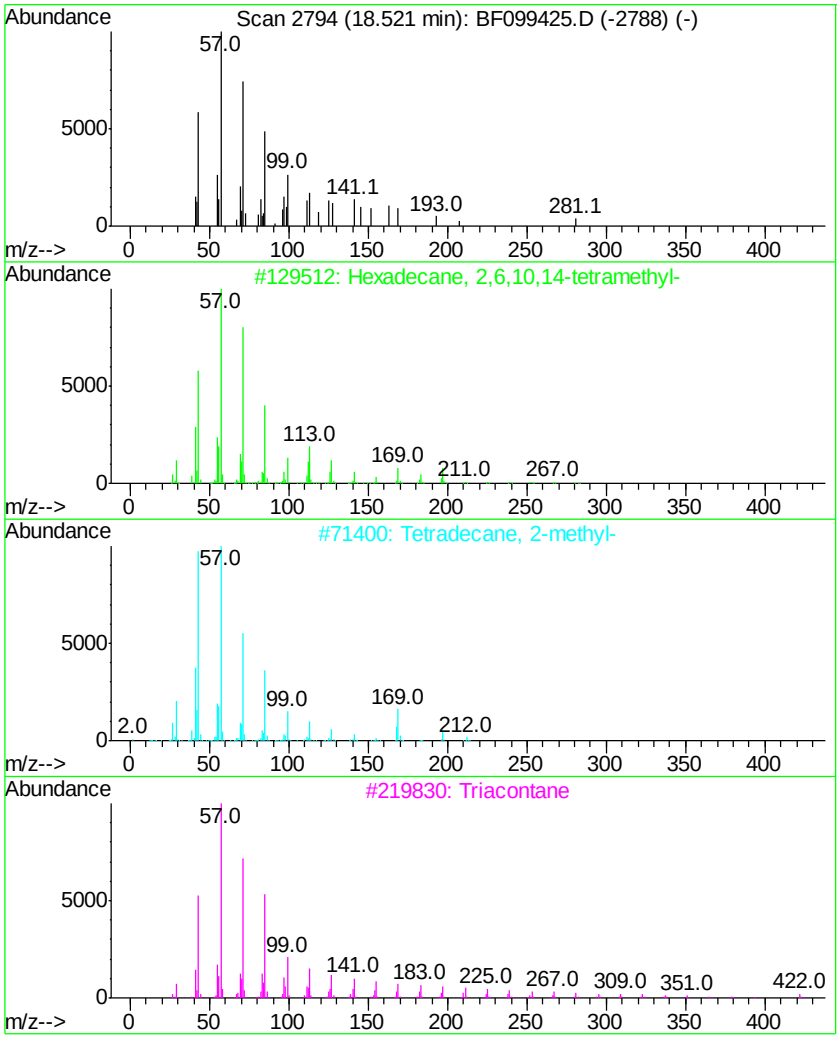
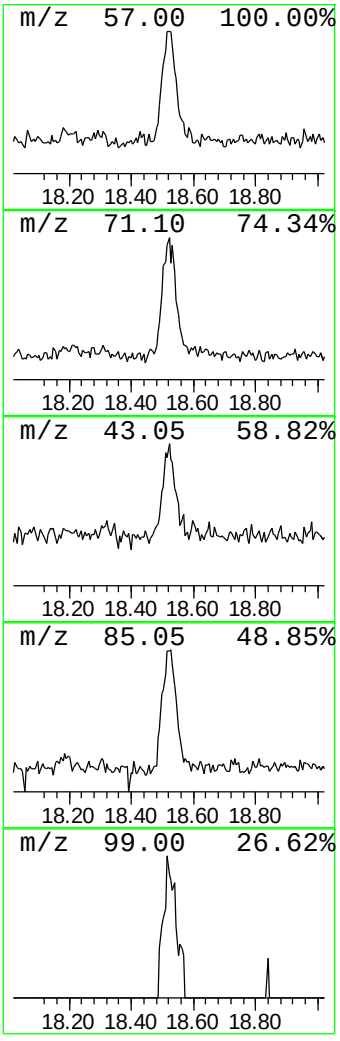
Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.52	2.55 ng	68582	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	59
2	Tetradecane, 2-methyl-	212	C15H32	001560-95-8	59
3	Triacontane	422	C30H62	000638-68-6	59
4	Heptacosane	380	C27H56	000593-49-7	53
5	Hentriacontane	437	C31H64	000630-04-6	52





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF101217\
Data File : BF099425.D
Acq On : 13 Oct 2017 6:58
Operator : SJ/JU
Sample : I5731-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100417-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	2.13	9.3	ng	289025	1	6.85	624547	20.0
2-Pentanone, 4-hy...	5.07	5.4	ng	168657	1	6.85	624547	20.0
unknown6.62	6.62	53.4	ng	1666890	1	6.85	624547	20.0
Heneicosane	15.91	4.5	ng	121826	6	15.49	536987	20.0
Octacosane	16.41	5.3	ng	143257	6	15.49	536987	20.0
Pentacosane	17.69	3.9	ng	104118	6	15.49	536987	20.0
Hexadecane, 2,6,1...	18.52	2.5	ng	68582	6	15.49	536987	20.0