LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108463.D
Acq On : 24 Aug 2018 15:08
Operator : JU/SJ
Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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	2.437	13	17	24	rVB	82185	120935	2.59%	0.321%
2	5.266	494	498	507	rBV	112522	152115	3.26%	0.404%
3	5.637	556	561	564	rBV	3300151	3351980	71.90%	8.900%
4	6.625	723	729	732	rBV	3381836	3545422	76.05%	9.414%
5	6.772	749	754	757	rBV	3544417	3548270	76.11%	9.422%
6	7.001	789	793	796	rBV	1056833	955366	20.49%	2.537%
7	7.154	815	819	823	rBV	2813293	2832497	60.76%	7.521%
8	7.560	882	888	892	rBV	2016590	2372307	50.89%	6.299%
9	8.284	1005	1011	1014	rBV	1286354	1206335	25.88%	3.203%
10	9.360	1187	1194	1197	rBV	4480368	4524666	97.06%	12.014%
11	10.042	1304	1310	1324	rBV	1451179	1486460	31.89%	3.947%
12	10.842	1439	1446	1467	rBV	2713586	2837830	60.88%	7.535%
13	11.542	1559	1565	1568	rBV	1791416	1580720	33.91%	4.197%
14	13.130	1830	1835	1838	rBV	4906302	4661732	100.00%	12.378%
15	14.195	2011	2016	2025	rBV	1140053	1123713	24.11%	2.984%
16	14.318	2033	2037	2042	rVB	62803	59627	1.28%	0.158%
17	14.624	2082	2089	2094	rBV	150400	178754	3.83%	0.475%
18	14.954	2139	2145	2150	rBV	334986	366165	7.85%	0.972%
19	15.313	2200	2206	2214	rVB	412591	524615	11.25%	1.393%
20	15.742	2269	2279	2289	rBV2	583890	1321858	28.36%	3.510%
21	16.201	2350	2357	2366	rVB	291916	465926	9.99%	1.237%
22	16.748	2444	2450	2459	rVB	137117	260773	5.59%	0.692%
23	17.395	2555	2560	2571	rVB3	51165	117965	2.53%	0.313%
24	18.171	2686	2692	2699	rVB5	24671	64908	1.39%	0.172%

Sum of corrected areas: 37660939

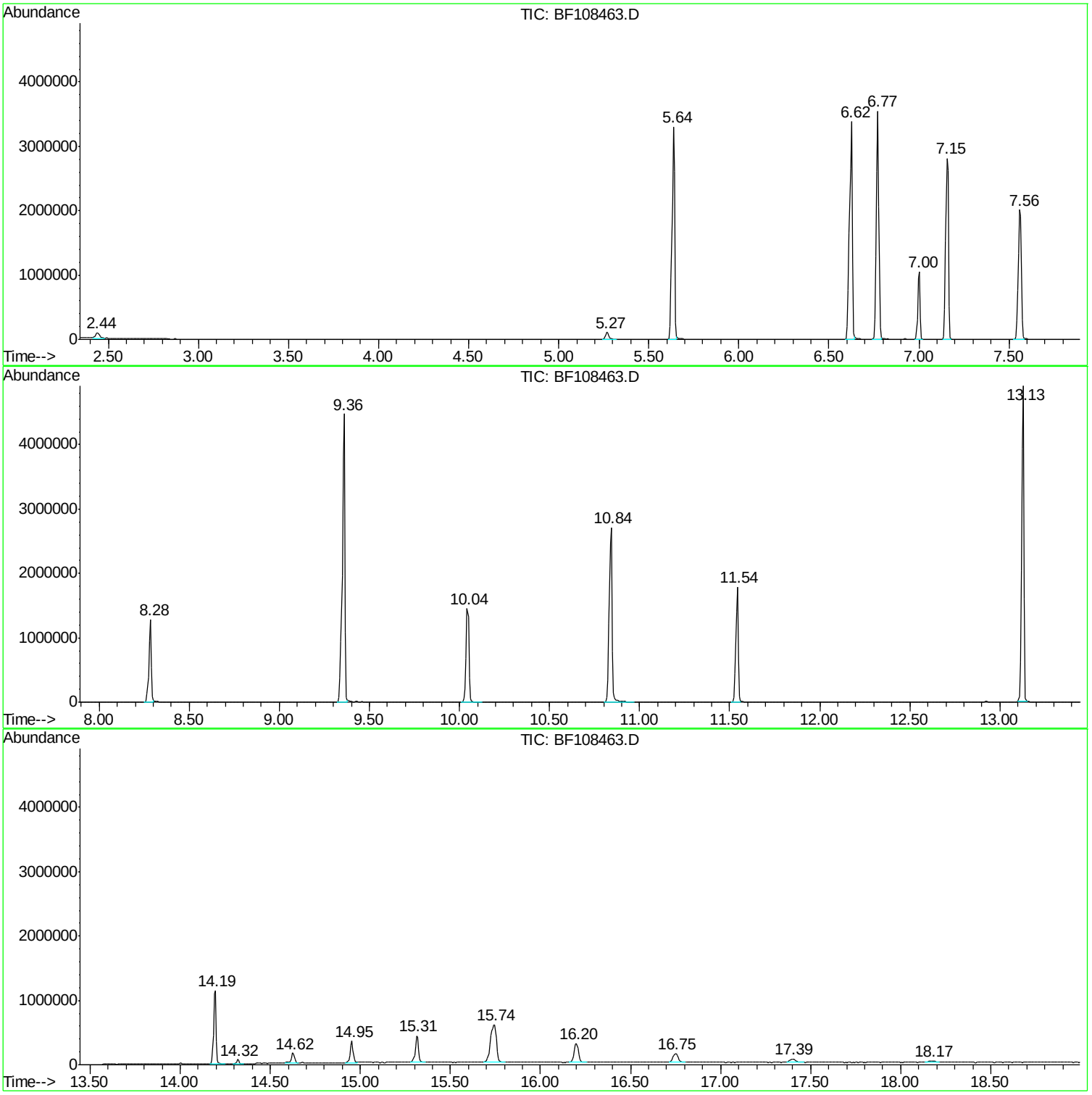
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108463.D
Acq On : 24 Aug 2018 15:08
Operator : JU/SJ
Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108463.D
Acq On : 24 Aug 2018 15:08
Operator : JU/SJ
Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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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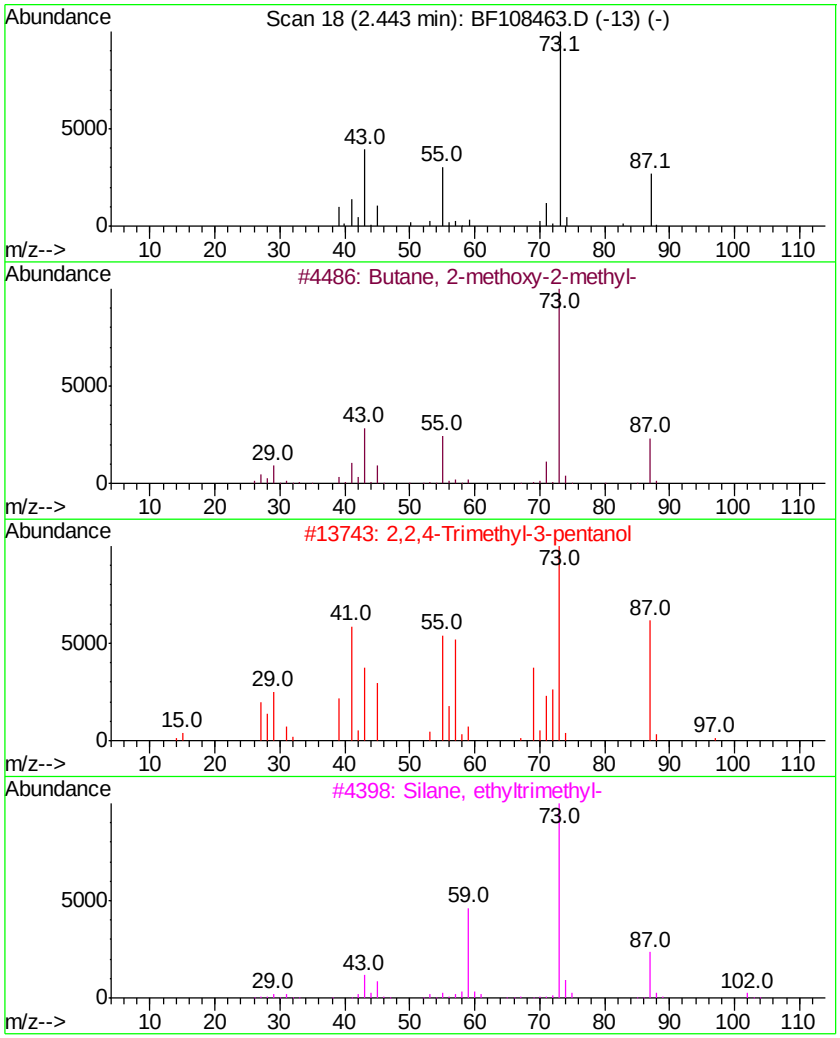
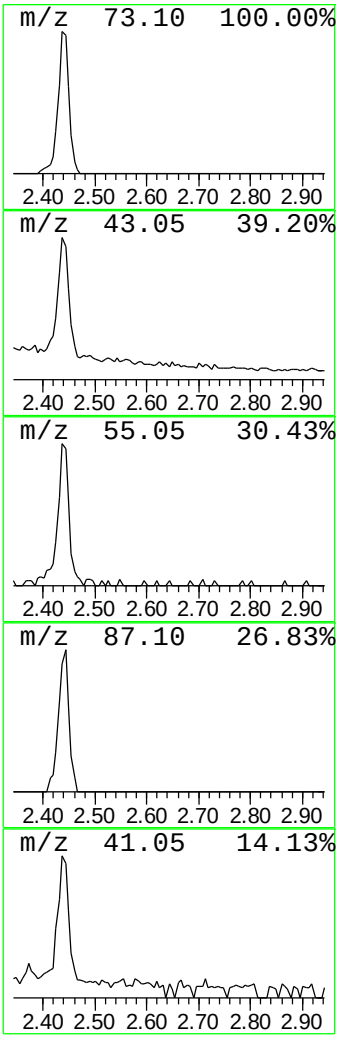
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	2.53 ng	120935	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108463.D
Acq On : 24 Aug 2018 15:08
Operator : JU/SJ
Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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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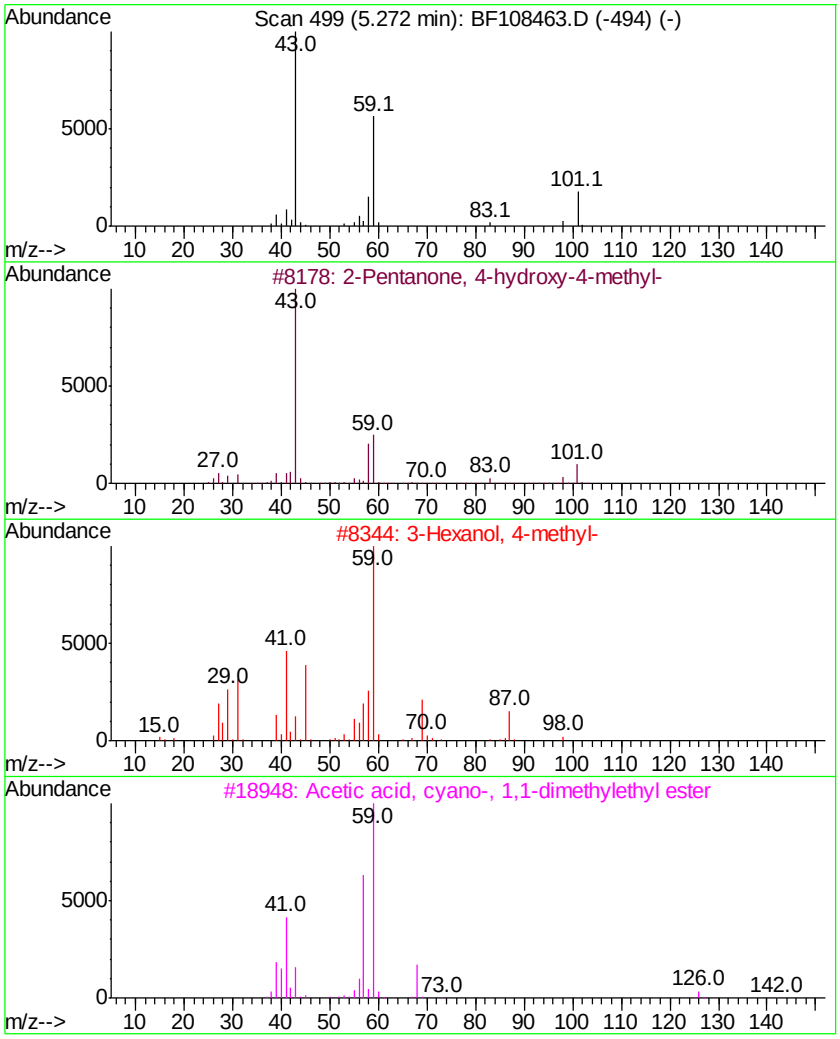
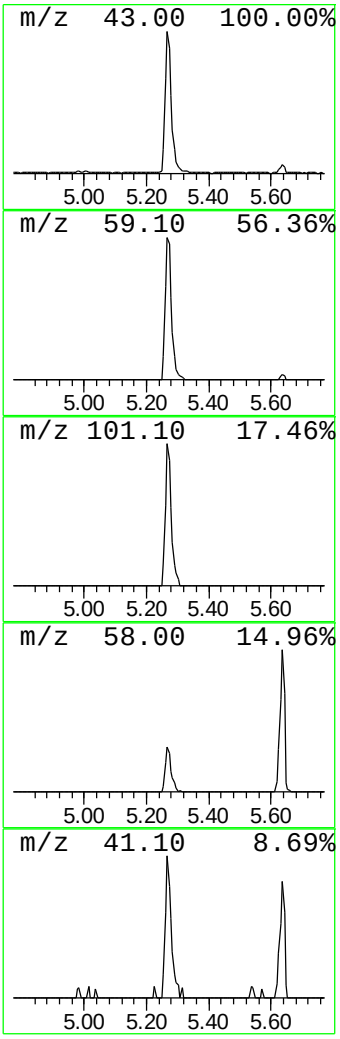
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	3.18 ng	152115	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	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108463.D
Acq On : 24 Aug 2018 15:08
Operator : JU/SJ
Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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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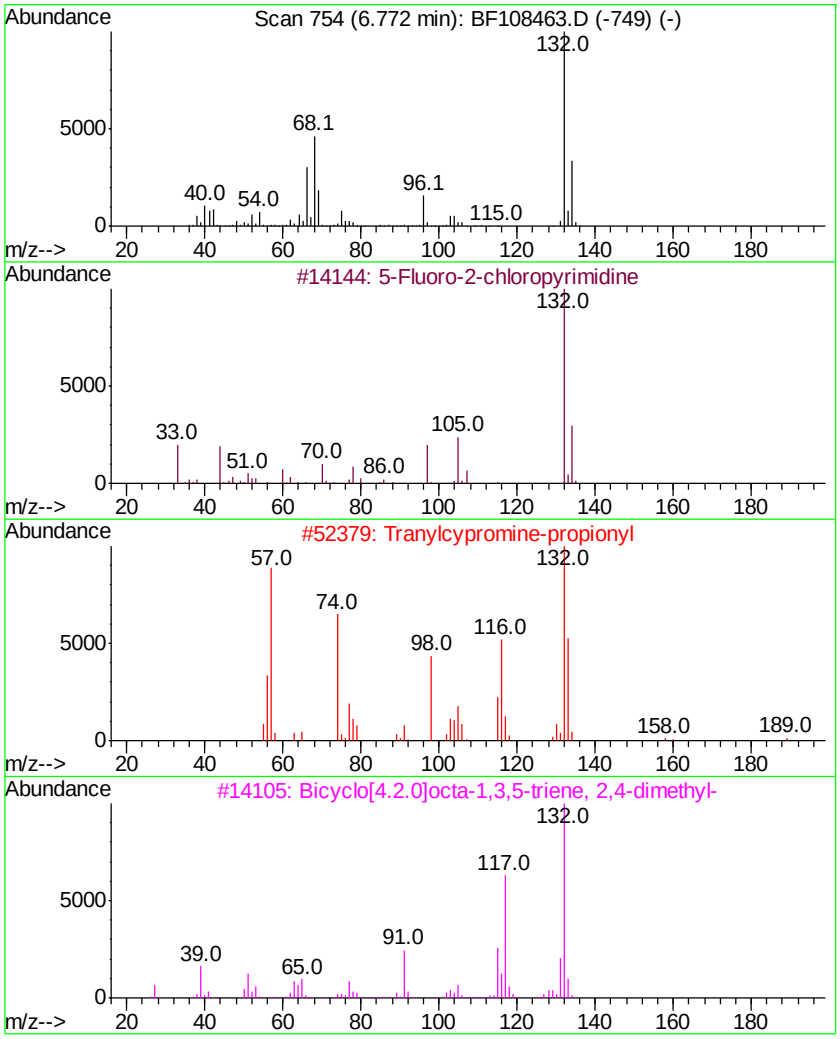
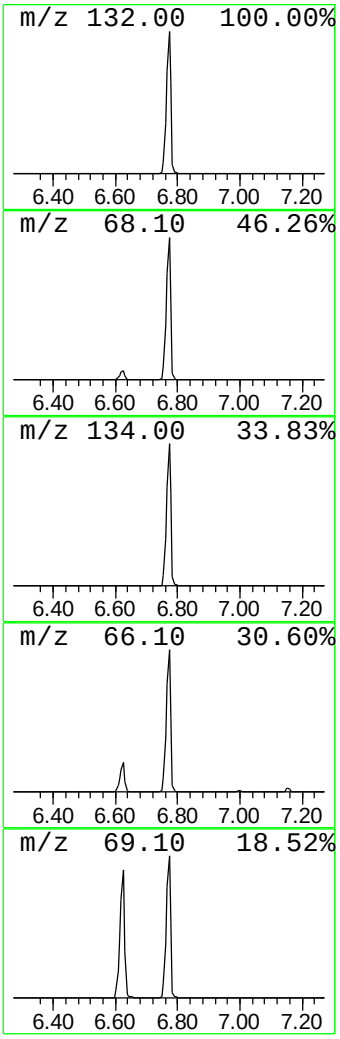
Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	74.28 ng	3548270	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108463.D
Acq On : 24 Aug 2018 15:08
Operator : JU/SJ
Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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

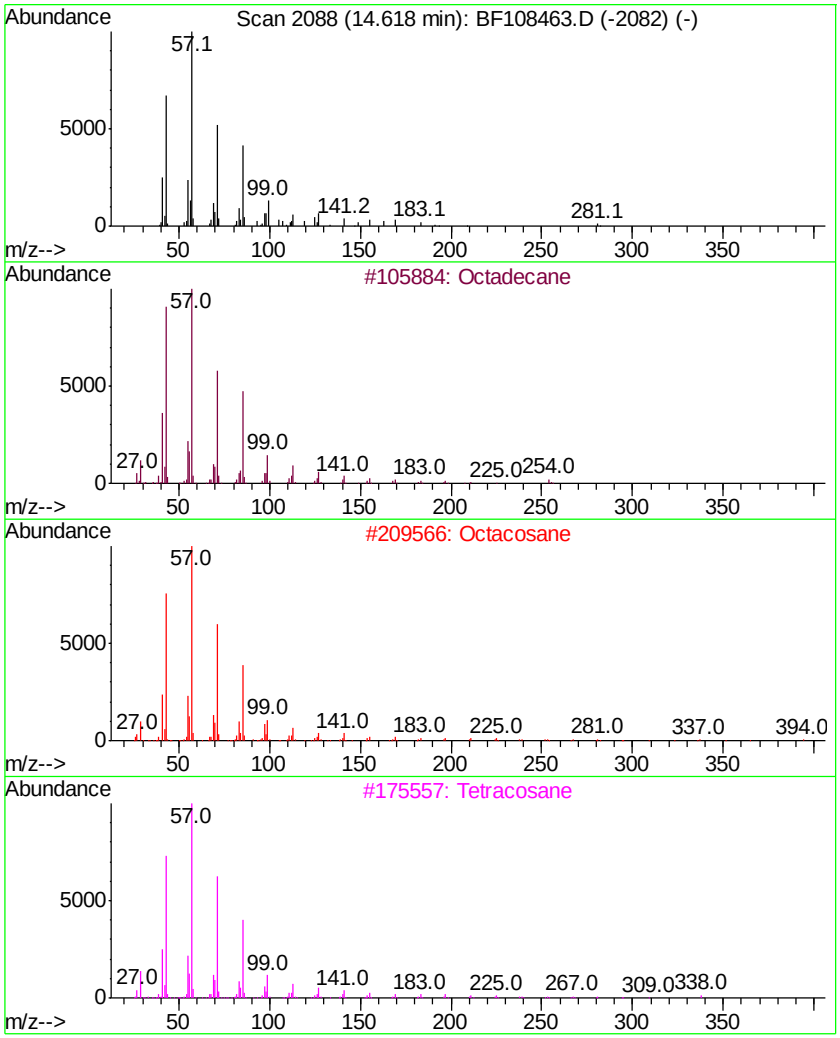
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

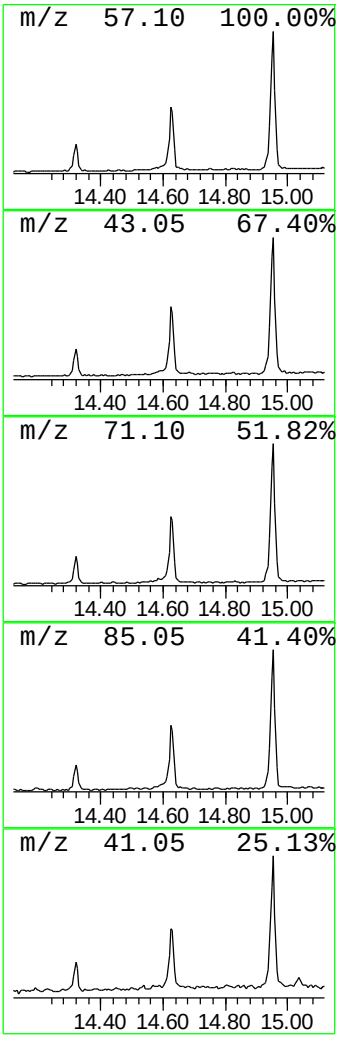
****

Peak Number 5 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.18 ng	178754	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108463.D
Acq On : 24 Aug 2018 15:08
Operator : JU/SJ
Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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

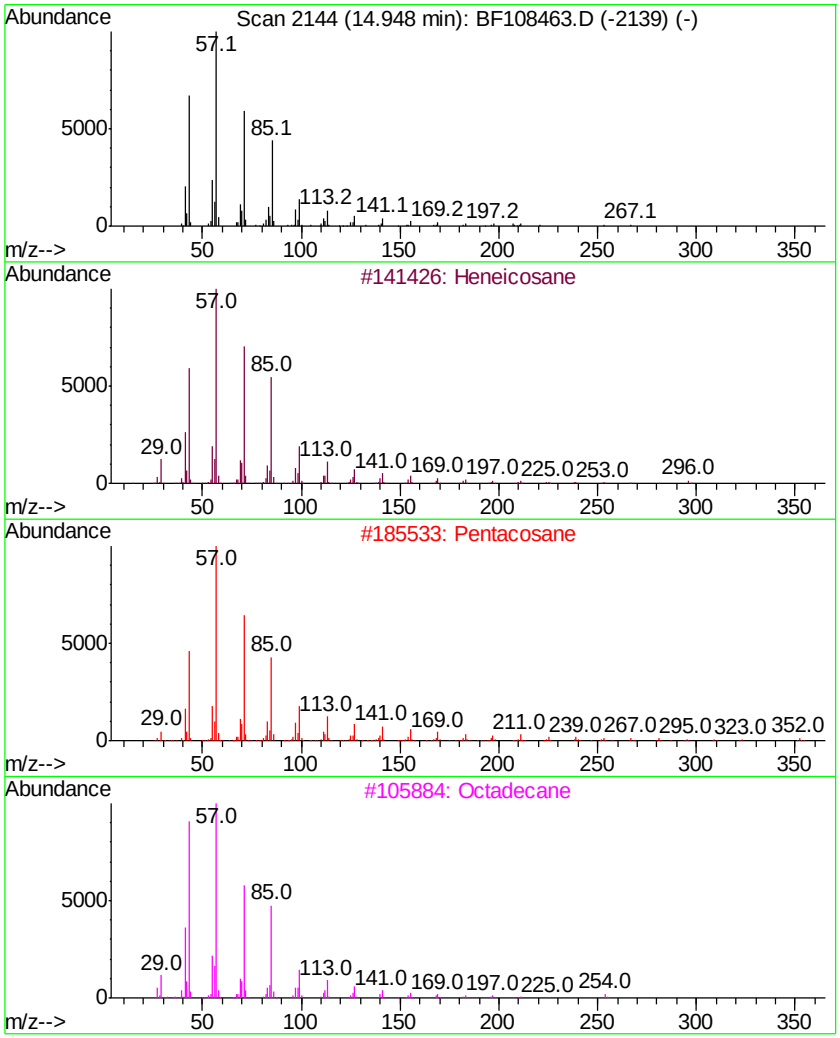
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

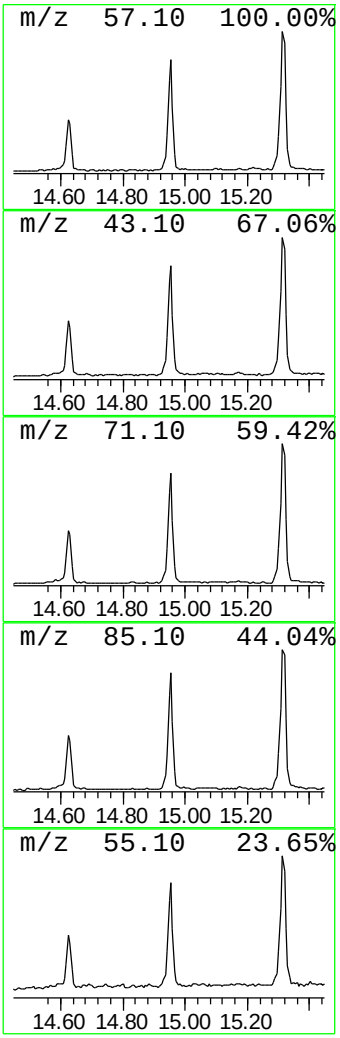
****

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	6.52 ng	366165	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

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Operator : JU/SJ
Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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

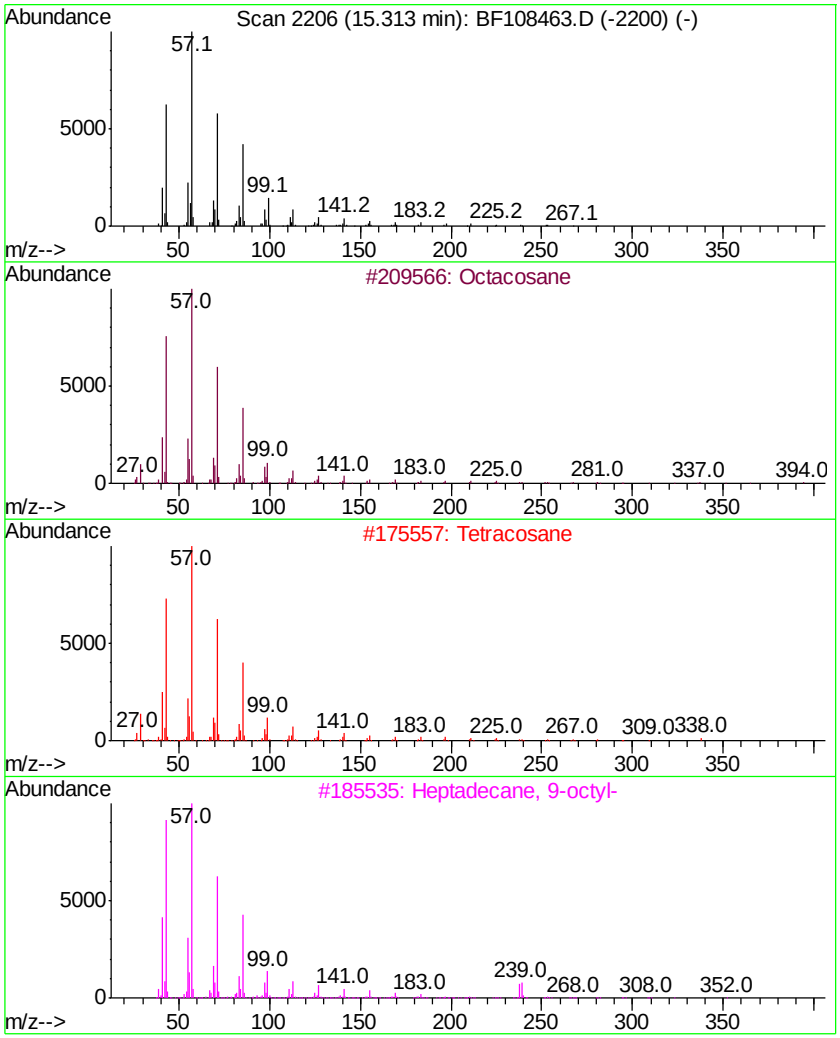
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

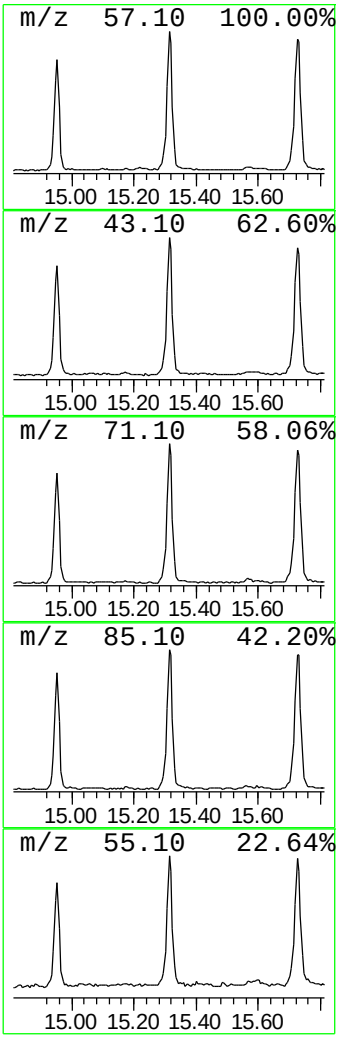
****

Peak Number 7 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	7.94 ng	524615	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

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Sample : PB112334BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

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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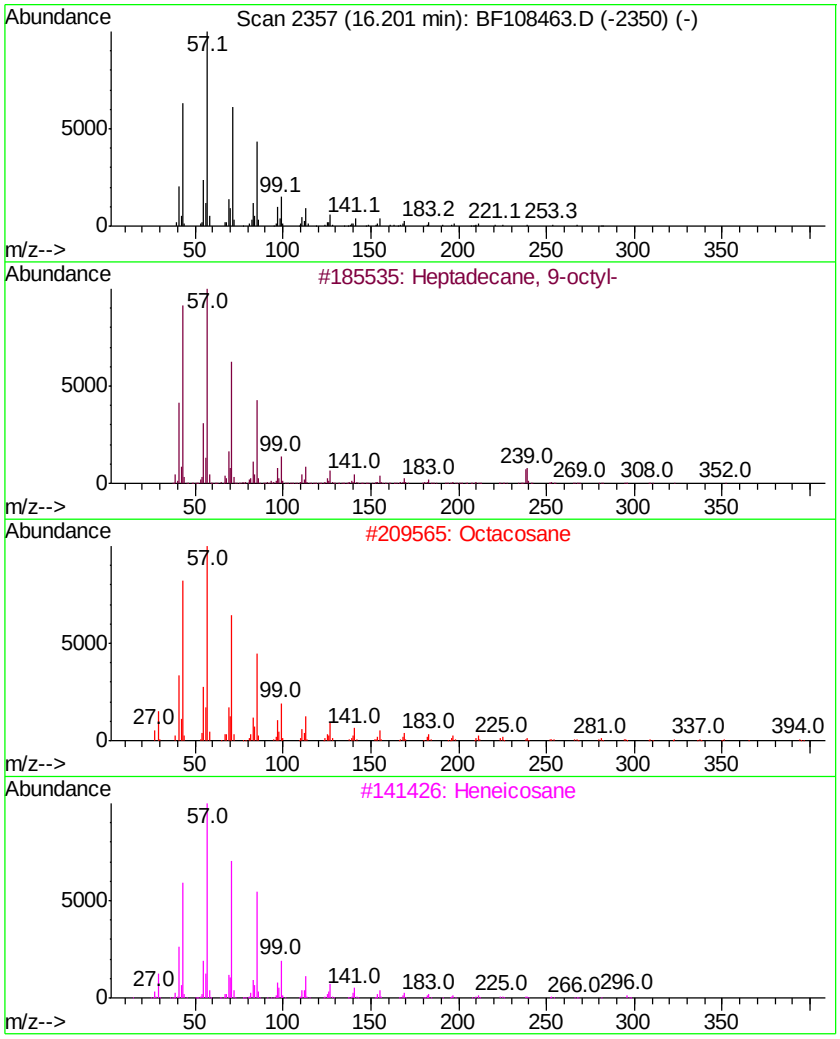
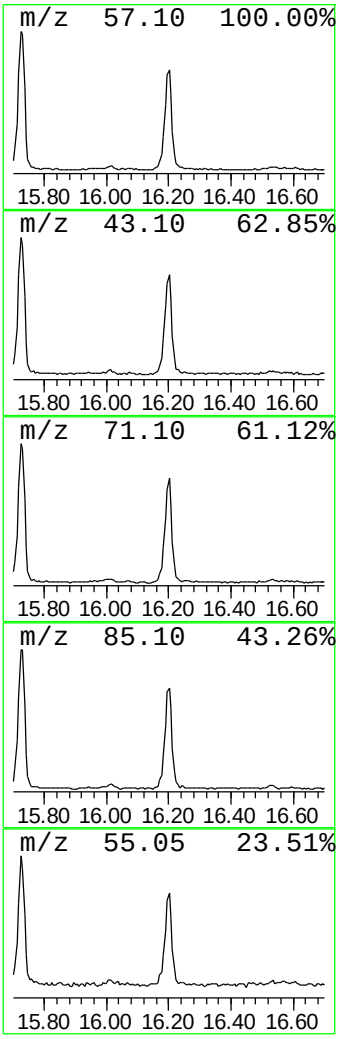
Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	7.05 ng	465926	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Tetracosane	338	C24H50	000646-31-1	91





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ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112334BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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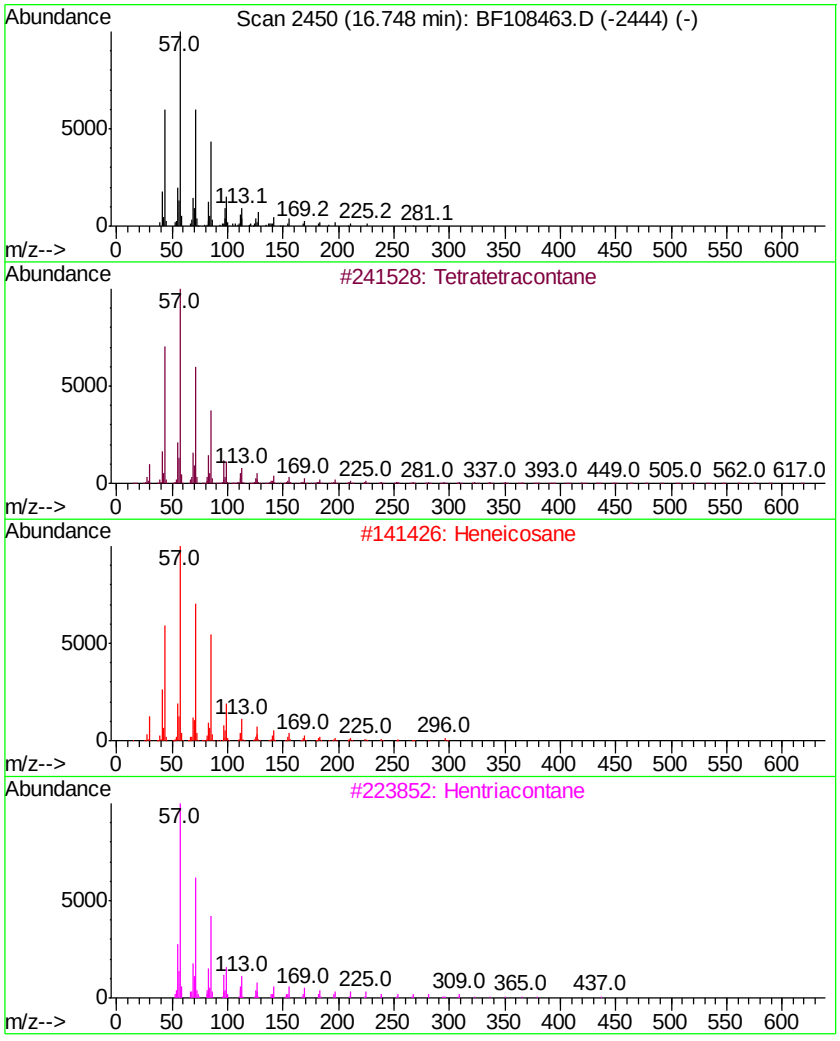
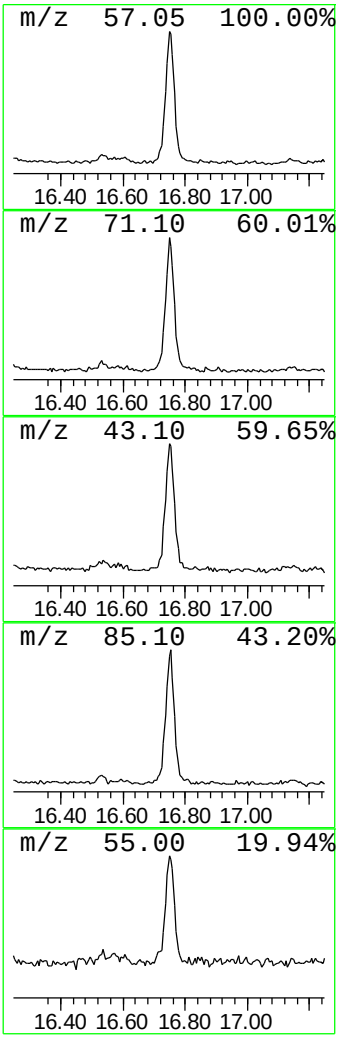
Peak Number 9 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	3.95 ng	260773	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082418\
Data File : BF108463.D
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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...	2.44	2.5	ng	120935	1	7.00	955366	20.0
2-Pentanone, 4-hy...	5.27	3.2	ng	152115	1	7.00	955366	20.0
unknown6.77	6.77	74.3	ng	3548270	1	7.00	955366	20.0
Octadecane	14.62	3.2	ng	178754	5	14.19	1123710	20.0
Heneicosane	14.95	6.5	ng	366165	5	14.19	1123710	20.0
Tetracosane	15.31	7.9	ng	524615	6	15.75	1321860	20.0
Heptadecane, 9-oc...	16.20	7.0	ng	465926	6	15.75	1321860	20.0
Tetratetracontane	16.75	4.0	ng	260773	6	15.75	1321860	20.0