LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108545.D
Acq On : 28 Aug 2018 7:45
Operator : JU/SJ
Sample : J4660-01
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-D-B

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	5.231	489	492	503	rVB	62999	66642	1.85%	0.326%
2	5.625	555	559	578	rVB	1125666	1067190	29.69%	5.227%
3	6.613	724	727	740	rBV	848641	776581	21.60%	3.804%
4	6.766	749	753	757	rBV	2114435	1889600	52.56%	9.255%
5	7.001	789	793	796	rBV	703795	642218	17.86%	3.146%
6	7.154	815	819	823	rBV	2713874	2613912	72.71%	12.803%
7	7.566	883	889	892	rBV	2029608	2100094	58.42%	10.286%
8	8.283	1007	1011	1027	rBV	775102	724456	20.15%	3.548%
9	9.354	1189	1193	1197	rBV	3869089	3594894	100.00%	17.607%
10	9.742	1256	1259	1272	rVB	59702	62143	1.73%	0.304%
11	9.977	1296	1299	1303	rBV	60142	69219	1.93%	0.339%
12	10.042	1307	1310	1324	rVB	788940	681215	18.95%	3.337%
13	10.701	1418	1422	1426	rVB	58012	47328	1.32%	0.232%
14	10.836	1441	1445	1457	rBV	1117633	1118256	31.11%	5.477%
15	11.536	1560	1564	1572	rBV	643976	580407	16.15%	2.843%
16	13.124	1829	1834	1837	rBV	3231443	2818971	78.42%	13.807%
17	14.077	1988	1996	2004	rBV9	23662	91822	2.55%	0.450%
18	14.189	2011	2015	2025	rVB	758059	690593	19.21%	3.382%
19	14.948	2141	2144	2148	rBV	43266	40707	1.13%	0.199%
20	15.030	2155	2158	2162	rBV	34713	37404	1.04%	0.183%
21	15.312	2202	2206	2213	rVB	48930	58560	1.63%	0.287%
22	15.742	2271	2279	2287	rBV	332398	523177	14.55%	2.562%
23	16.195	2351	2356	2363	rBV2	44075	68371	1.90%	0.335%
24	16.742	2444	2449	2456	rBV3	29866	53159	1.48%	0.260%

Sum of corrected areas: 20416919

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
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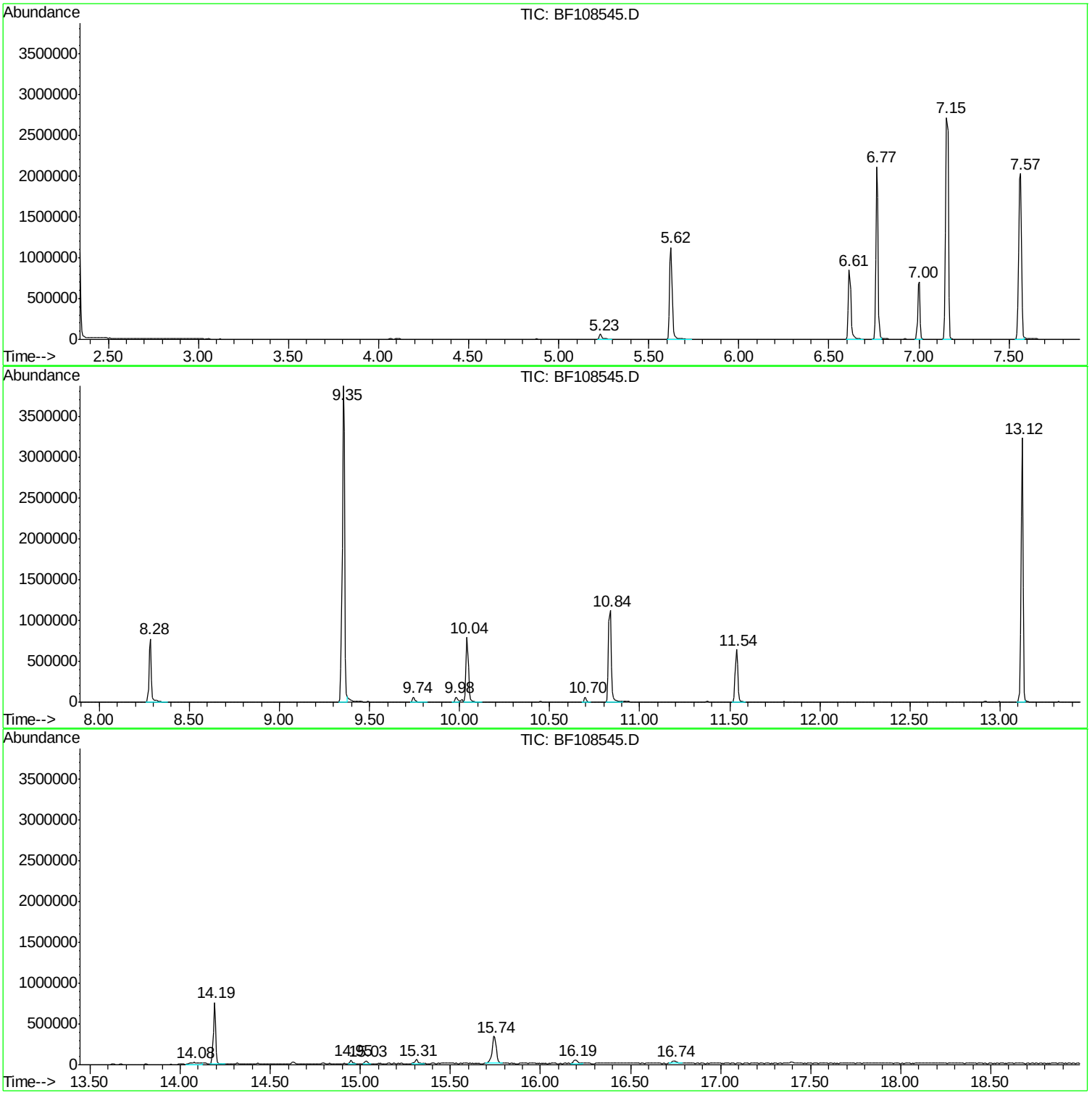
Operator : JU/SJ
Sample : J4660-01
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-D-B

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\BF082718\
Data File : BF108545.D
Acq On : 28 Aug 2018 7:45
Operator : JU/SJ
Sample : J4660-01
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-D-B

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

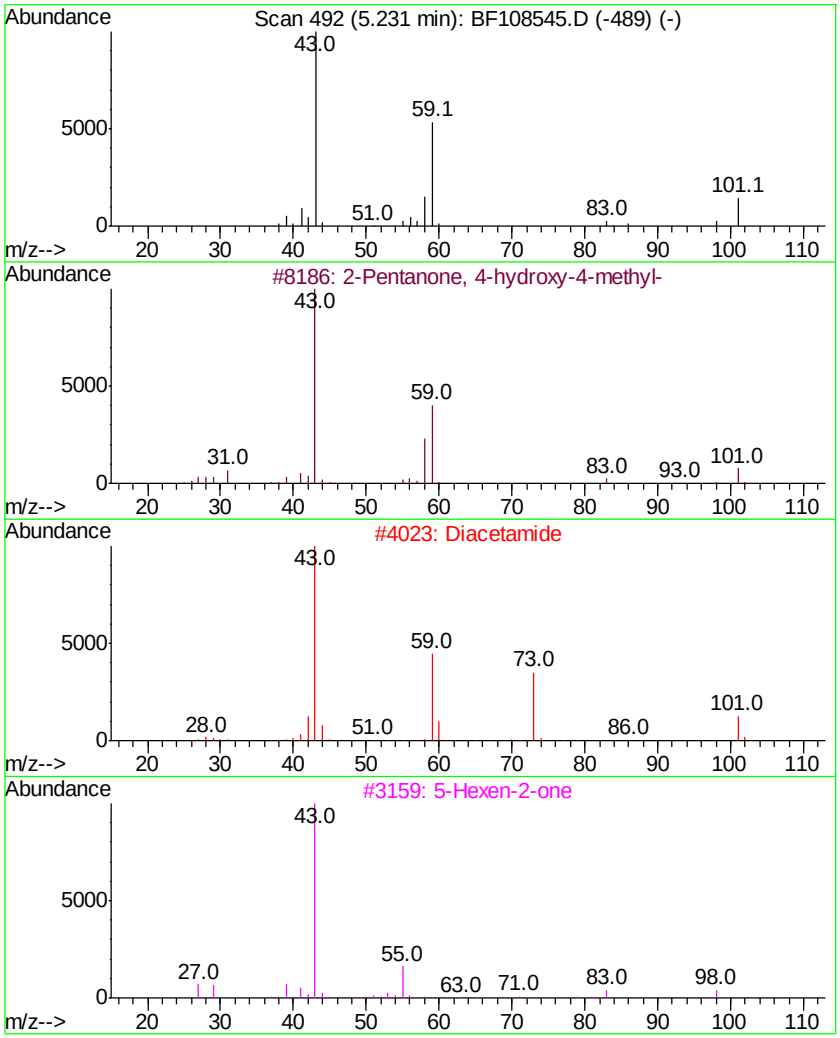
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

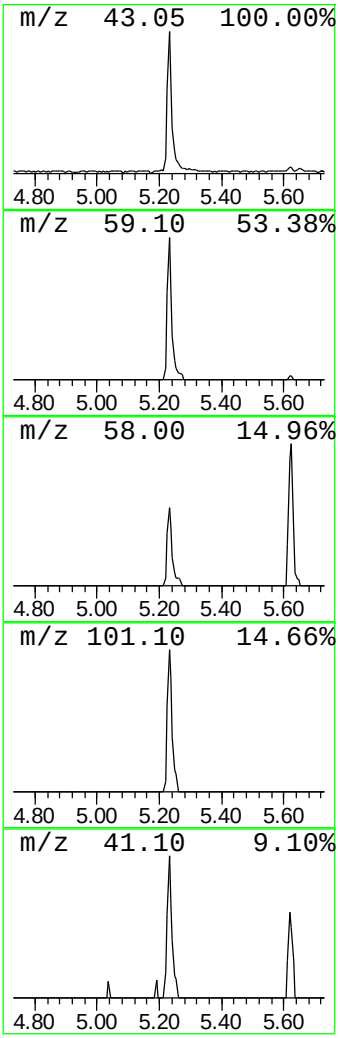
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	2.08 ng	66642	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	Diacetamide	101	C4H7NO2	000625-77-4	9
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Library Search Compound Report

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Data File : BF108545.D
Acq On : 28 Aug 2018 7:45
Operator : JU/SJ
Sample : J4660-01
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-D-B

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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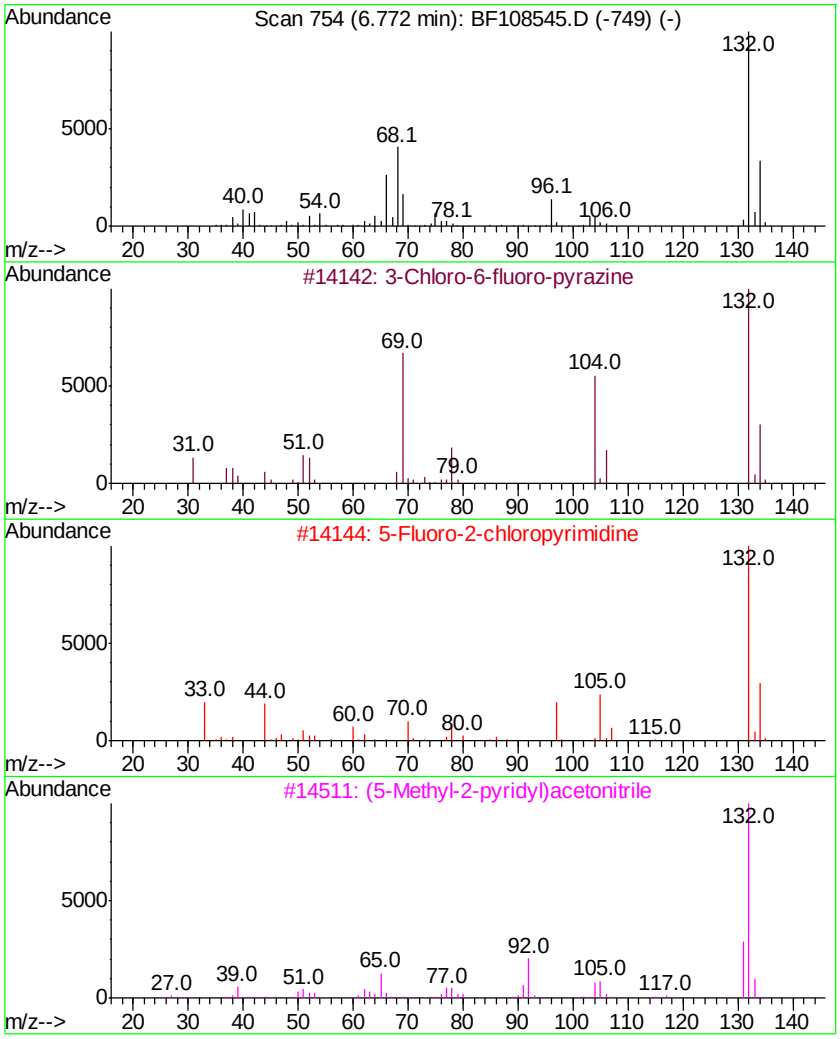
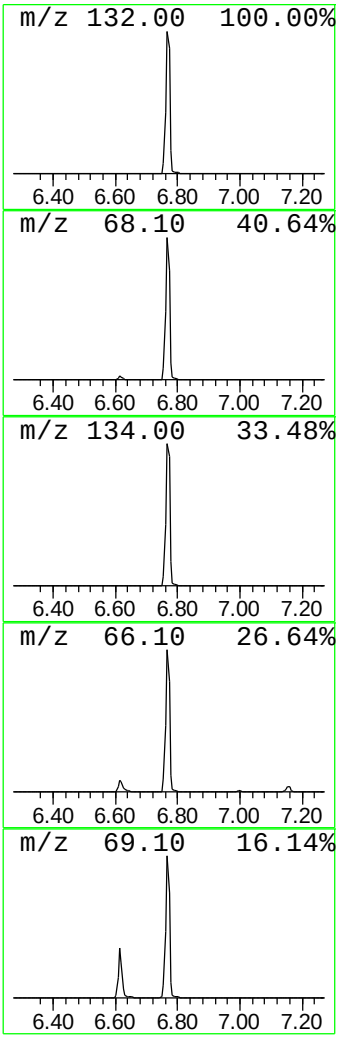
Peak Number 2 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	58.85 ng	1889600	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	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108545.D
Acq On : 28 Aug 2018 7:45
Operator : JU/SJ
Sample : J4660-01
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
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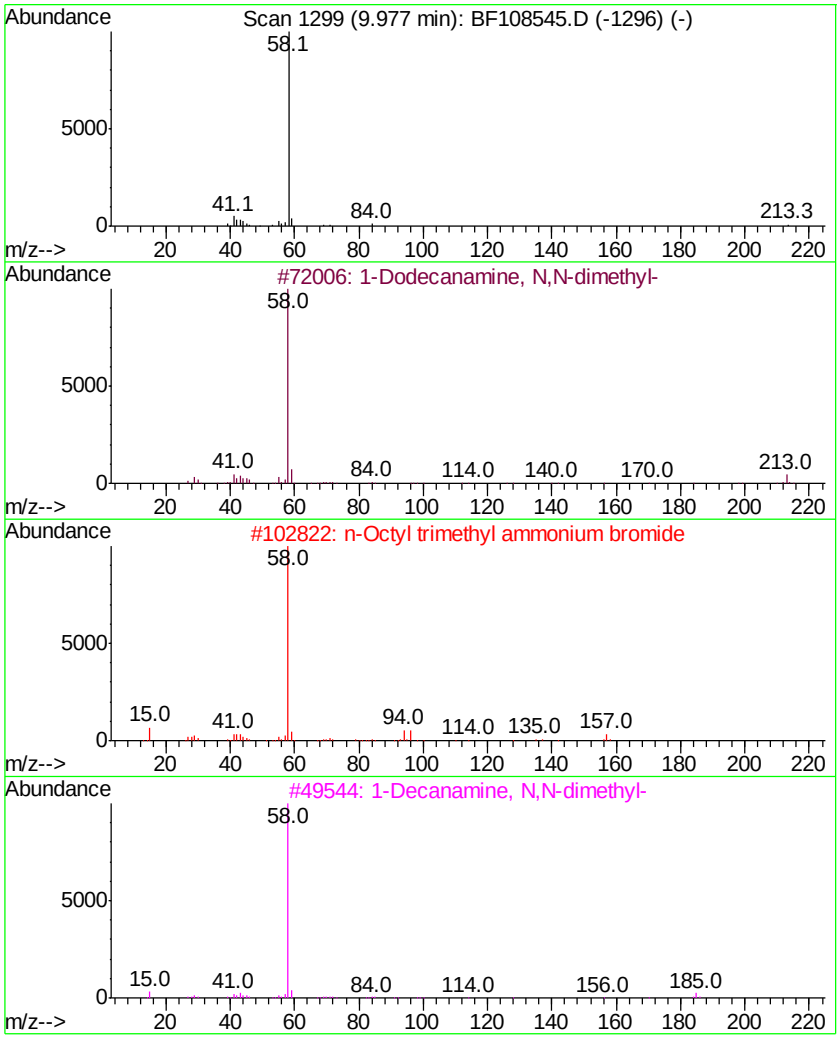
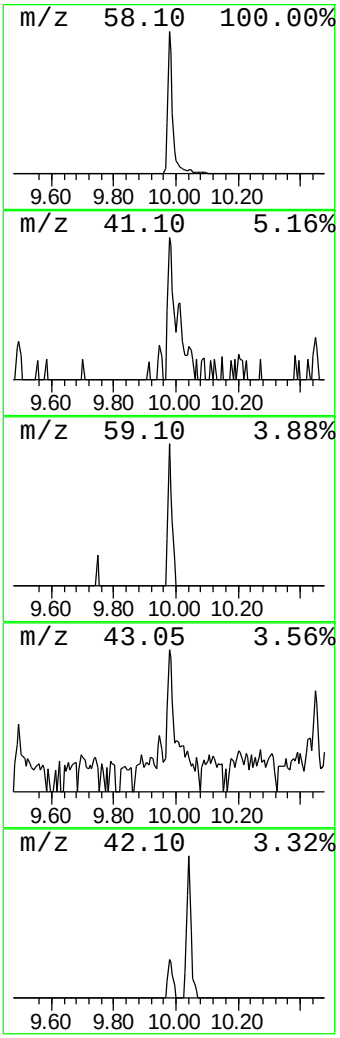
Peak Number 4 1-Dodecanamine, N,N-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.98	2.03 ng	69219	Acenaphthene-d10	10.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	80
2	n-Octyl trimethyl ammonium bromide	251	C11H26BrN	002083-68-3	78
3	1-Decanamine, N,N-dimethyl-	185	C12H27N	001120-24-7	74
4	1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	74
5	1-Tridecanamine, N,N-dimethyl-	227	C15H33N	017373-29-4	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108545.D
Acq On : 28 Aug 2018 7:45
Operator : JU/SJ
Sample : J4660-01
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-D-B

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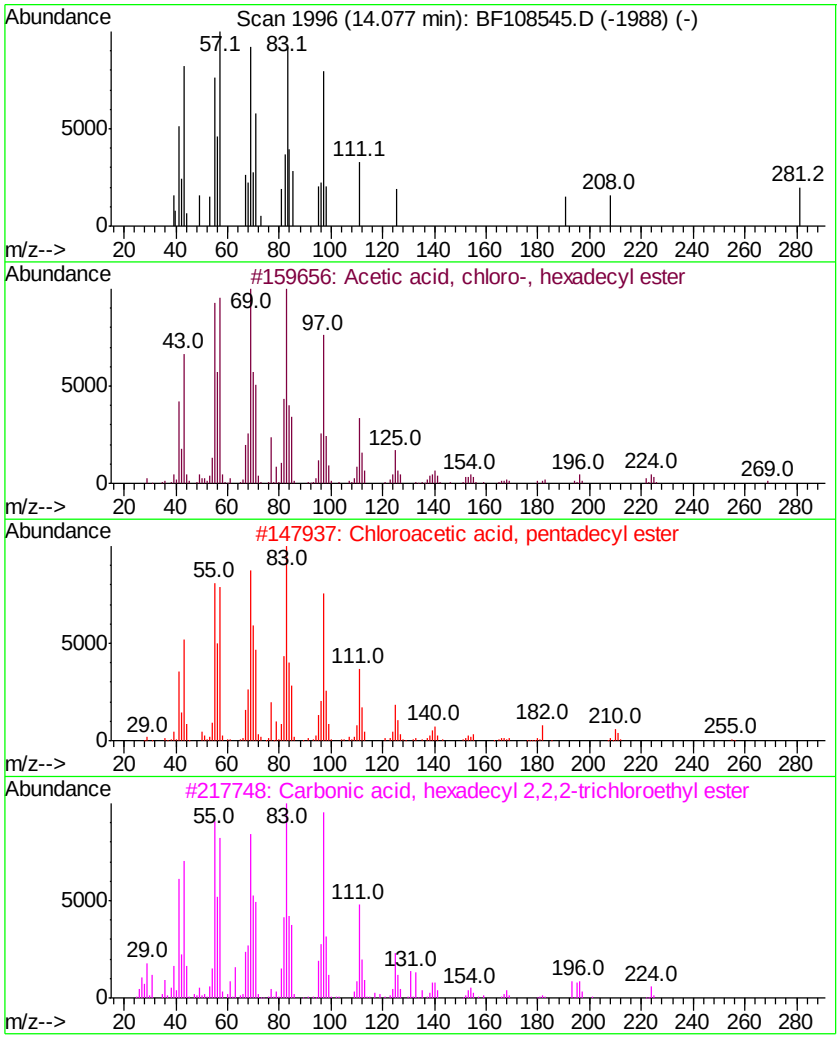
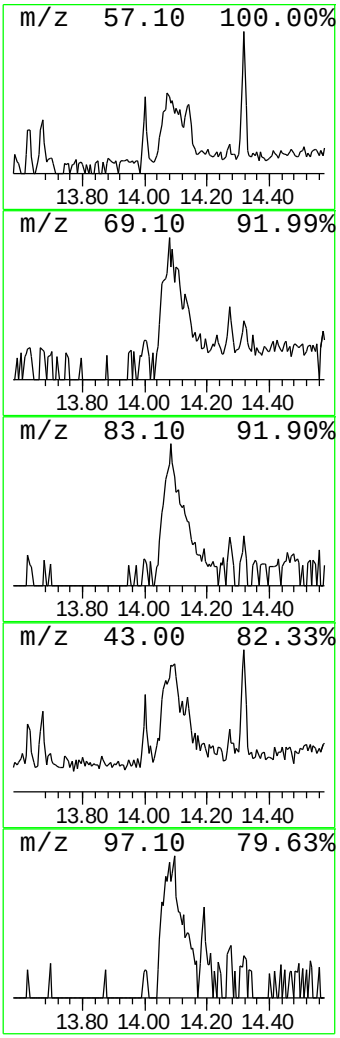
****

Peak Number 5 Acetic acid, chloro-, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	2.66 ng	91822	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	90
2	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	90
3	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	86
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
5	Carbonic acid, tridecyl 2,2,2-tr...	374	C16H29Cl3O3	1000314-55-9	80





Library Search Compound Report

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ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
082318-SIDI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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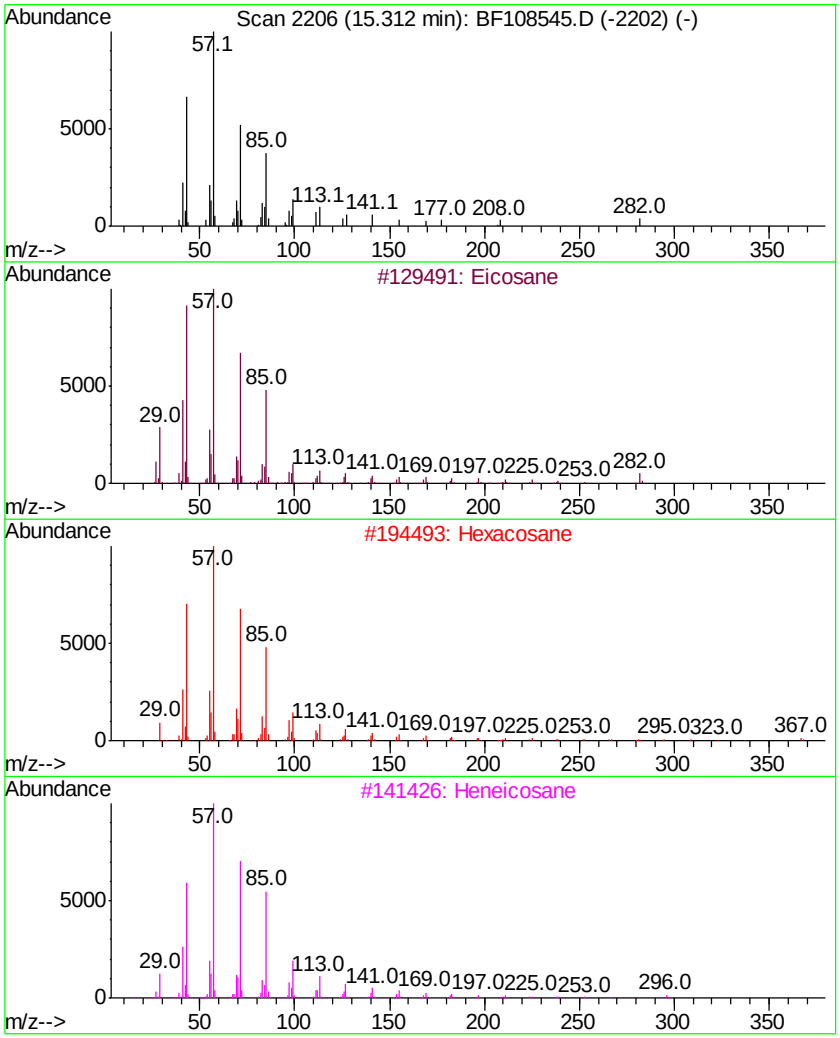
TIC Integration Parameters: LSCINT.P

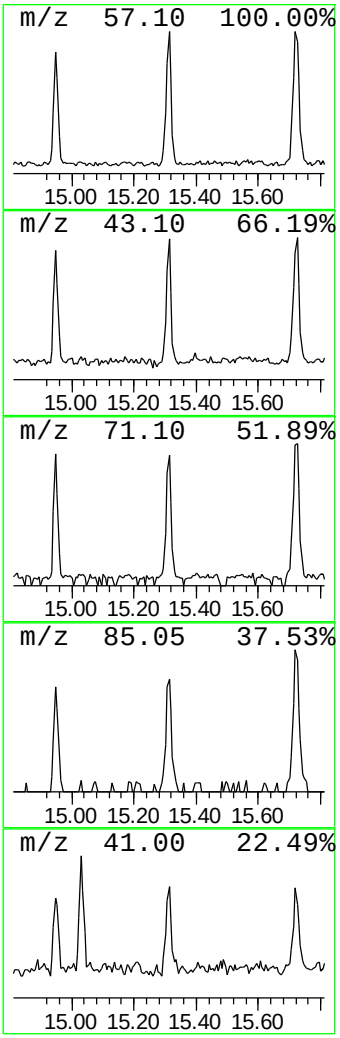
****

Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.24 ng	58560	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	99
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Heptacosane	380	C27H56	000593-49-7	90





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-D-B

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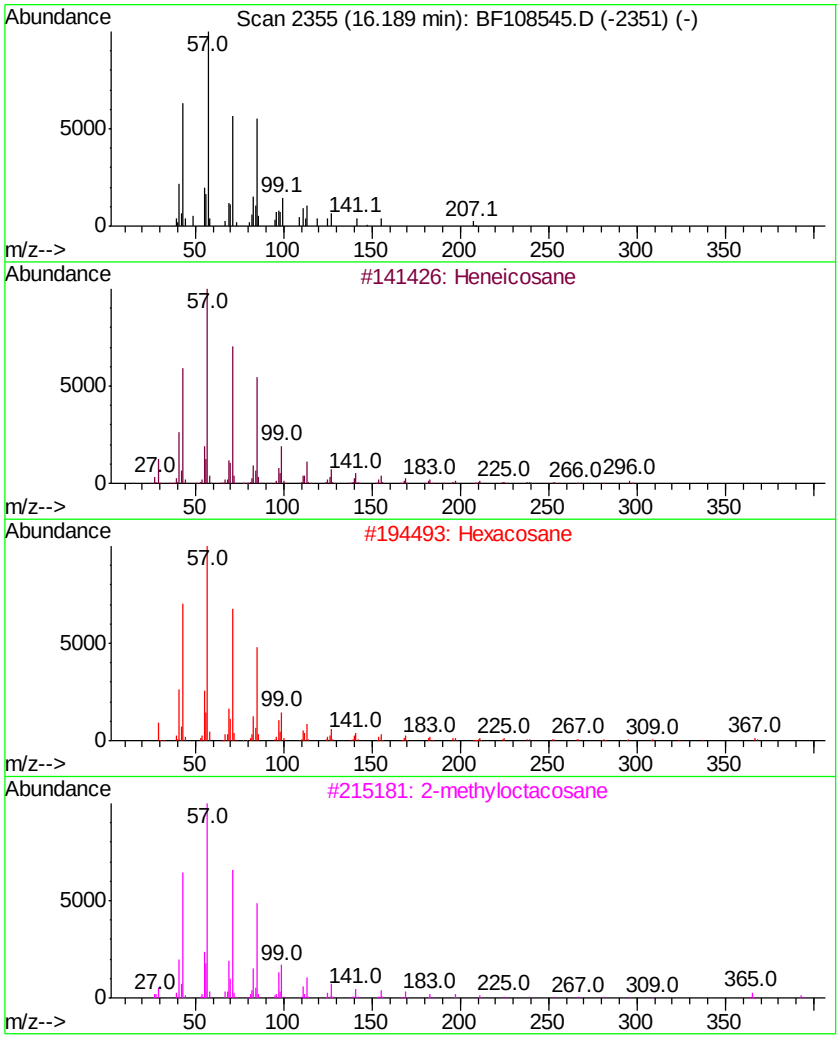
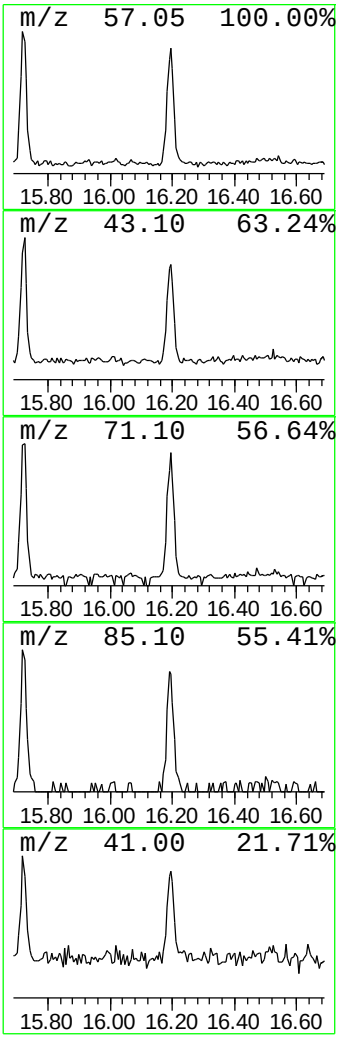
****

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.61 ng	68371	Perylene-d12	15.74

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





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

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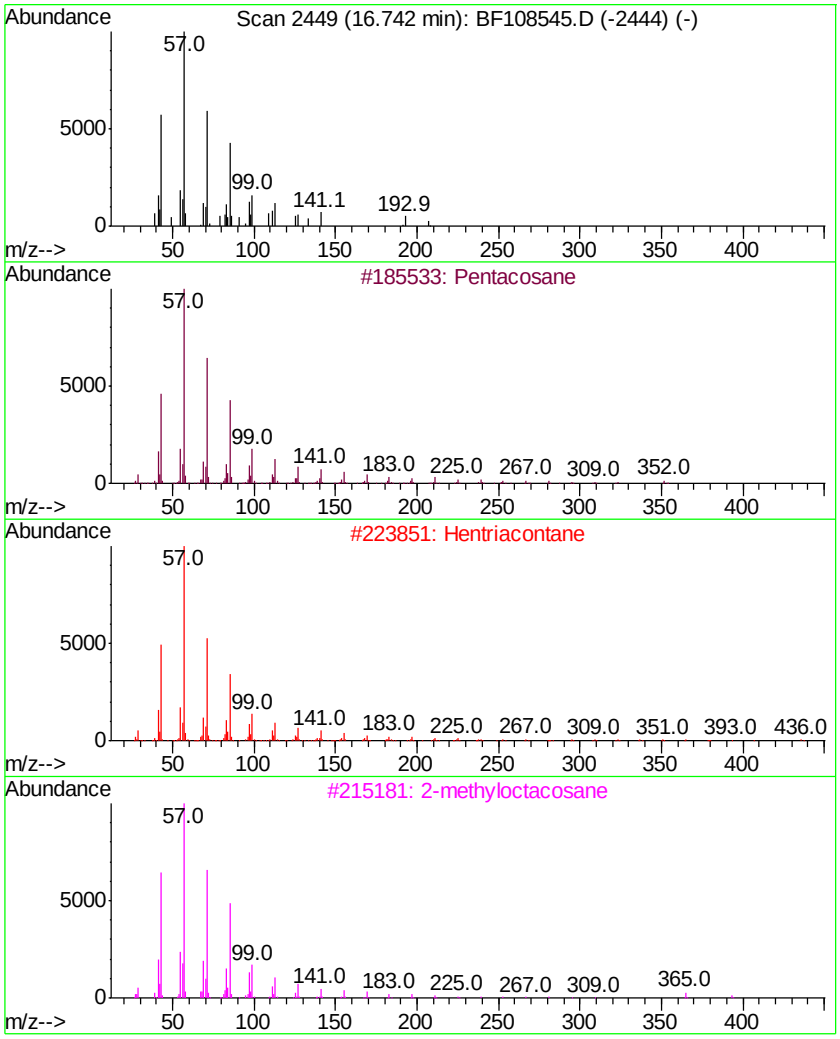
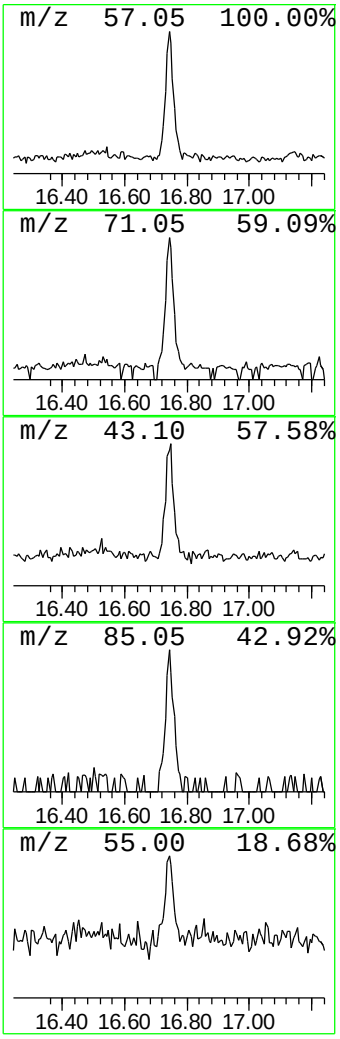
Peak Number 8 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	2.03 ng	53159	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	86
2	Hentriacontane	437	C31H64	000630-04-6	86
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Hexacosane	366	C26H54	000630-01-3	86
5	Tetracosane	338	C24H50	000646-31-1	80





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...	5.23	2.1	ng	66642	1	7.00	642218	20.0
unknown6.77	6.77	58.9	ng	1889600	1	7.00	642218	20.0
1-Dodecanamine, N...	9.98	2.0	ng	69219	3	10.04	681215	20.0
Acetic acid, chlo...	14.08	2.7	ng	91822	5	14.19	690593	20.0
Eicosane	15.31	2.2	ng	58560	6	15.74	523177	20.0
Heneicosane	16.19	2.6	ng	68371	6	15.74	523177	20.0
Pentacosane	16.74	2.0	ng	53159	6	15.74	523177	20.0