LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110636.D
Acq On : 9 Nov 2018 19:20
Operator : JU/SJ
Sample : J5864-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OLDMANS-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-BF110818.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	2.287	28	34	46	rVB	90657	132266	5.05%	0.631%
2	5.193	525	528	537	rBV	49202	73400	2.81%	0.350%
3	5.569	587	592	595	rBV	2186289	2031760	77.65%	9.686%
4	6.569	757	762	782	rBV	1888763	2324825	88.85%	11.084%
5	6.716	782	787	790	rBV	2303329	2237978	85.53%	10.670%
6	6.945	822	826	833	rBV	484682	446484	17.06%	2.129%
7	7.098	848	852	868	rBV	1843331	1681827	64.27%	8.018%
8	7.510	917	922	925	rBV	1423320	1367616	52.27%	6.520%
9	8.228	1039	1044	1055	rBV	565541	588227	22.48%	2.804%
10	9.298	1220	1226	1229	rBV	2636786	2522809	96.41%	12.027%
11	9.692	1289	1293	1299	rBV	122181	113230	4.33%	0.540%
12	9.986	1338	1343	1353	rVB	727724	683656	26.13%	3.259%
13	10.781	1473	1478	1491	rBV	1567330	1522725	58.19%	7.260%
14	11.480	1593	1597	1605	rBV	794852	735232	28.10%	3.505%
15	13.063	1861	1866	1869	rBV	2733984	2616624	100.00%	12.475%
16	13.939	2011	2015	2030	rBV	150519	244244	9.33%	1.164%
17	14.127	2043	2047	2055	rBV	682019	673851	25.75%	3.213%
18	14.557	2117	2120	2123	rBV	37778	39946	1.53%	0.190%
19	14.874	2170	2174	2177	rBV	62762	64070	2.45%	0.305%
20	14.957	2185	2188	2192	rVB	36454	35864	1.37%	0.171%
21	15.227	2229	2234	2239	rVB	87305	103355	3.95%	0.493%
22	15.621	2296	2301	2303	rBV	100111	125442	4.79%	0.598%
23	15.657	2303	2307	2314	rVB	287481	389646	14.89%	1.858%
24	16.074	2372	2378	2383	rBV2	77273	122706	4.69%	0.585%
25	16.598	2463	2467	2474	rVB2	37382	66278	2.53%	0.316%
26	17.215	2569	2572	2581	rVB4	15102	31311	1.20%	0.149%

Sum of corrected areas: 20975372

LSC Report - Integrated Chromatogram

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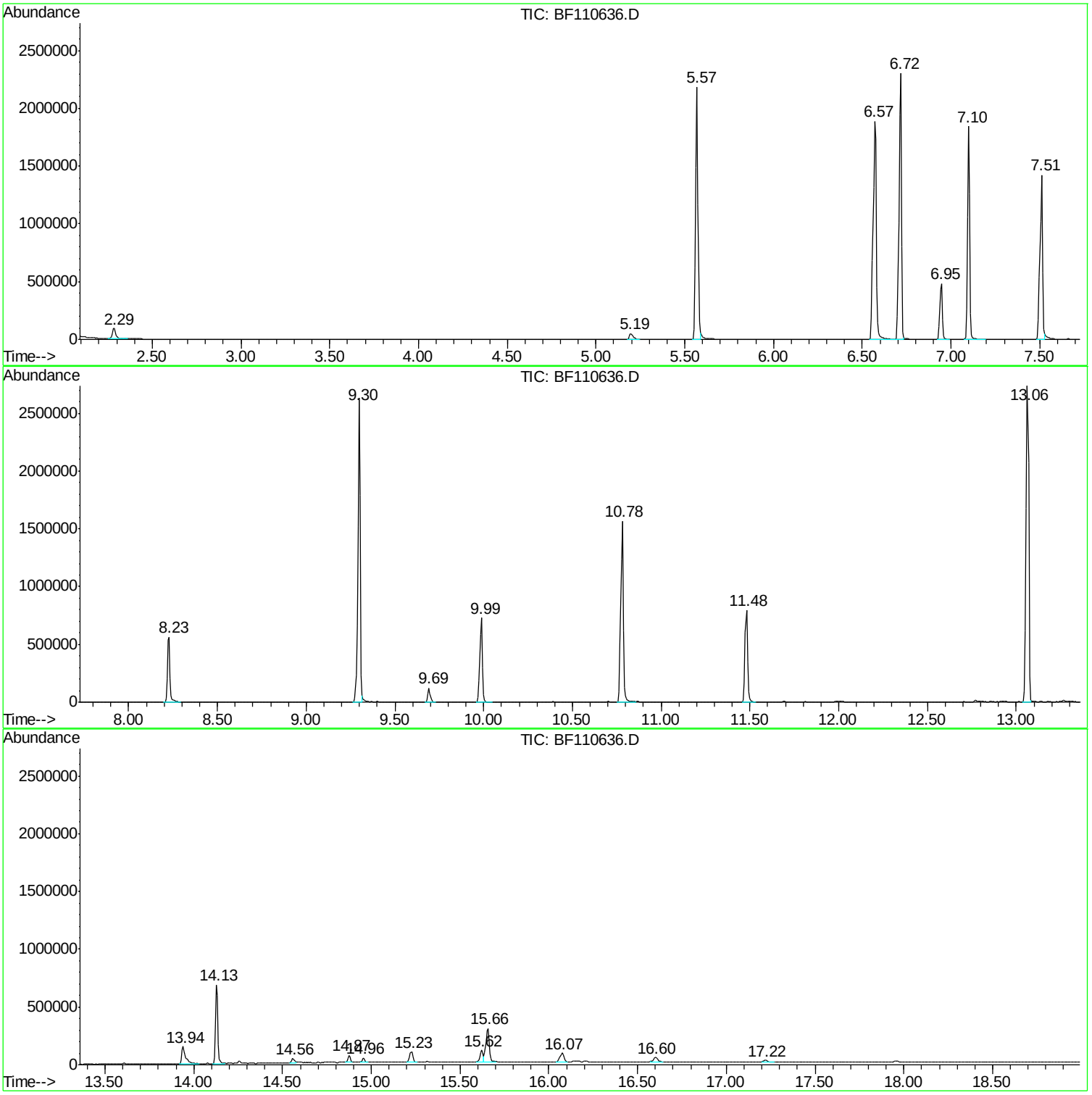
Sample : J5864-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OLDMANS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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\BF110918\
Data File : BF110636.D
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : OLDMANS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

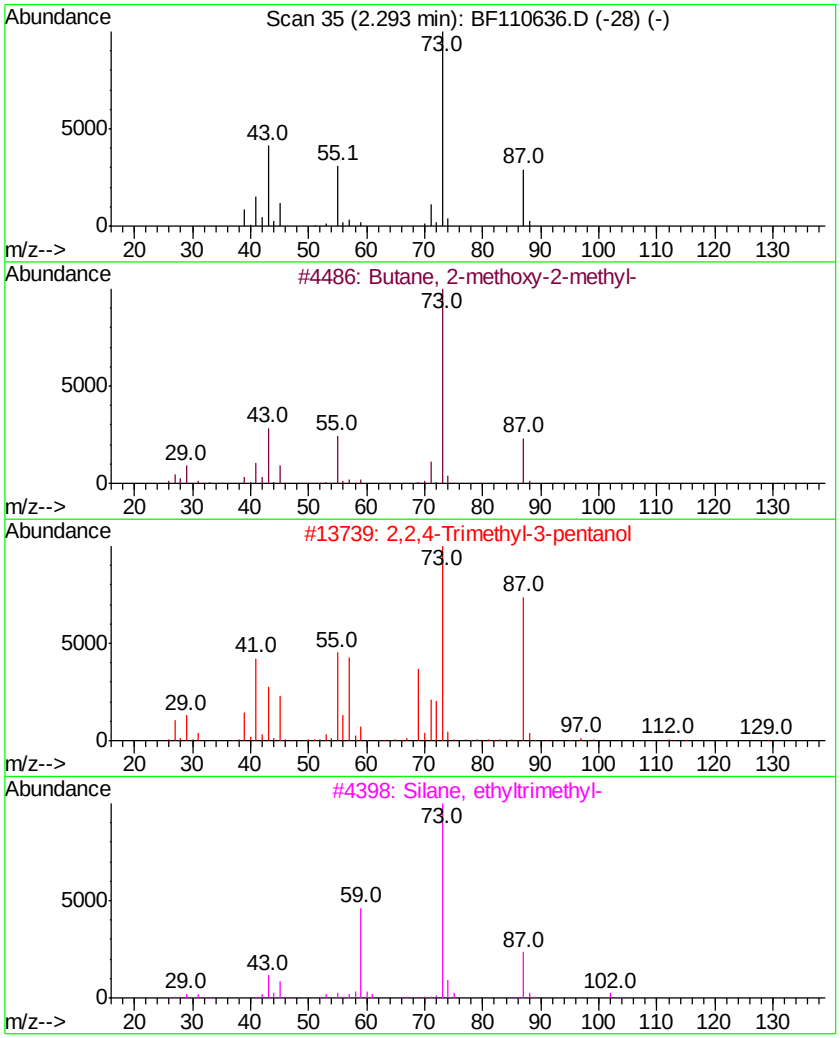
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

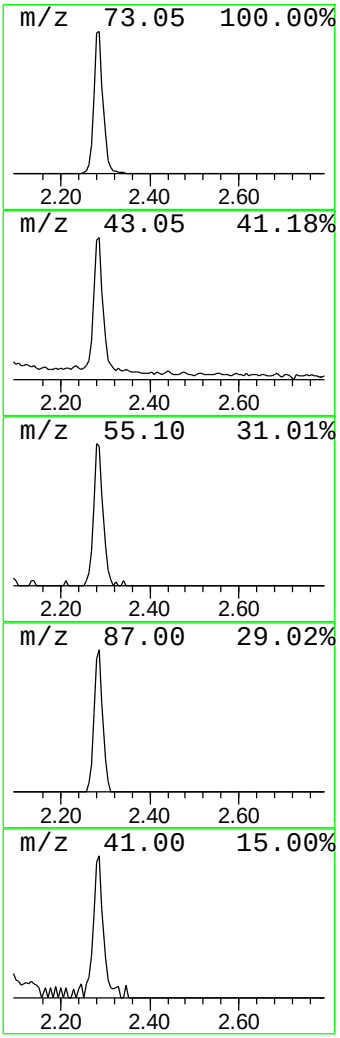
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	5.92 ng	132266	1,4-Dichlorobenzene-d4	6.95

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	39
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF110636.D
Acq On : 9 Nov 2018 19:20
Operator : JU/SJ
Sample : J5864-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OLDMANS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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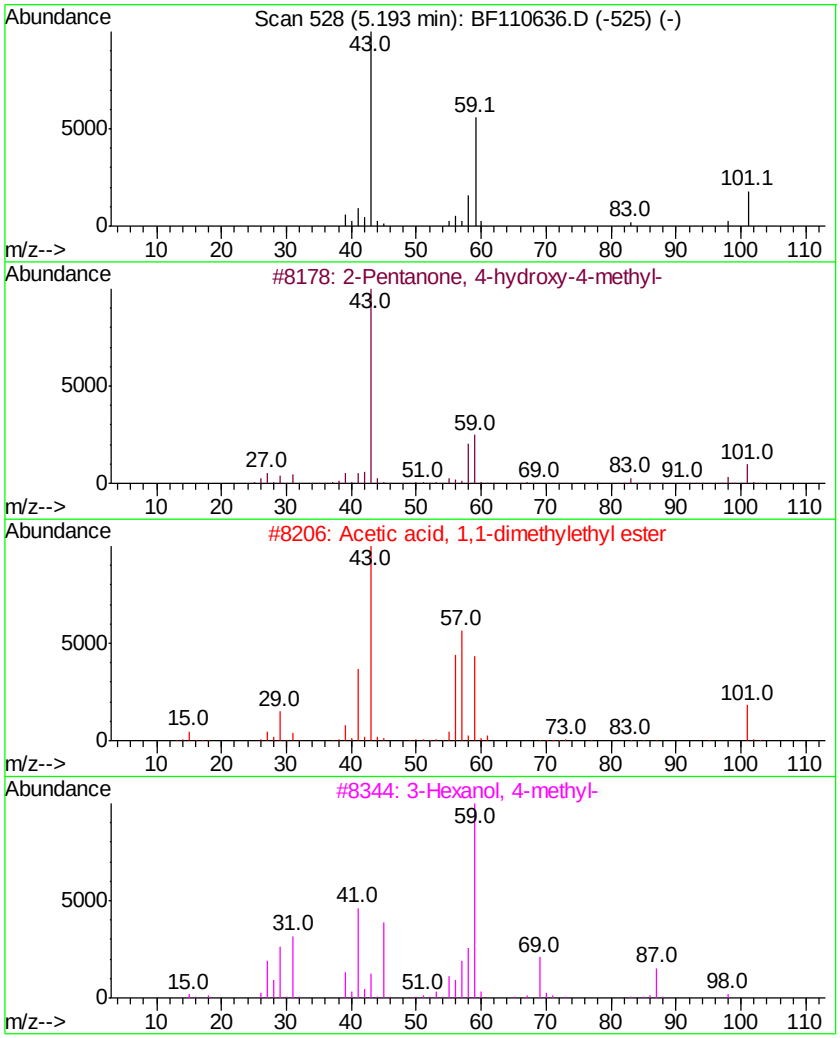
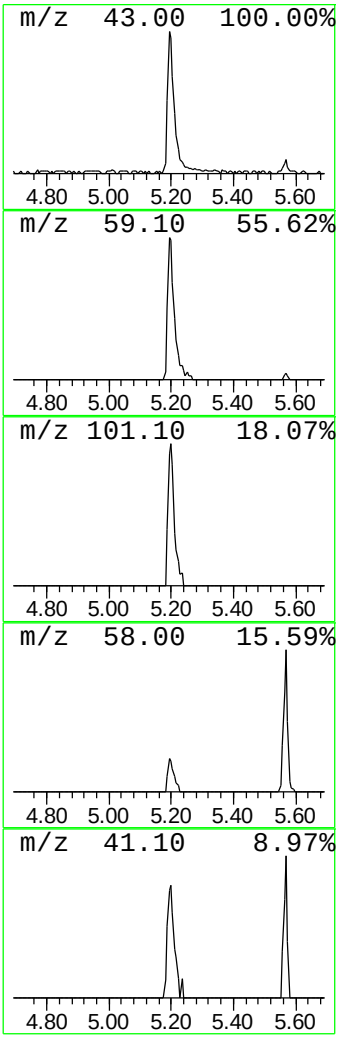
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.29 ng	73400	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110636.D
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Operator : JU/SJ
Sample : J5864-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OLDMANS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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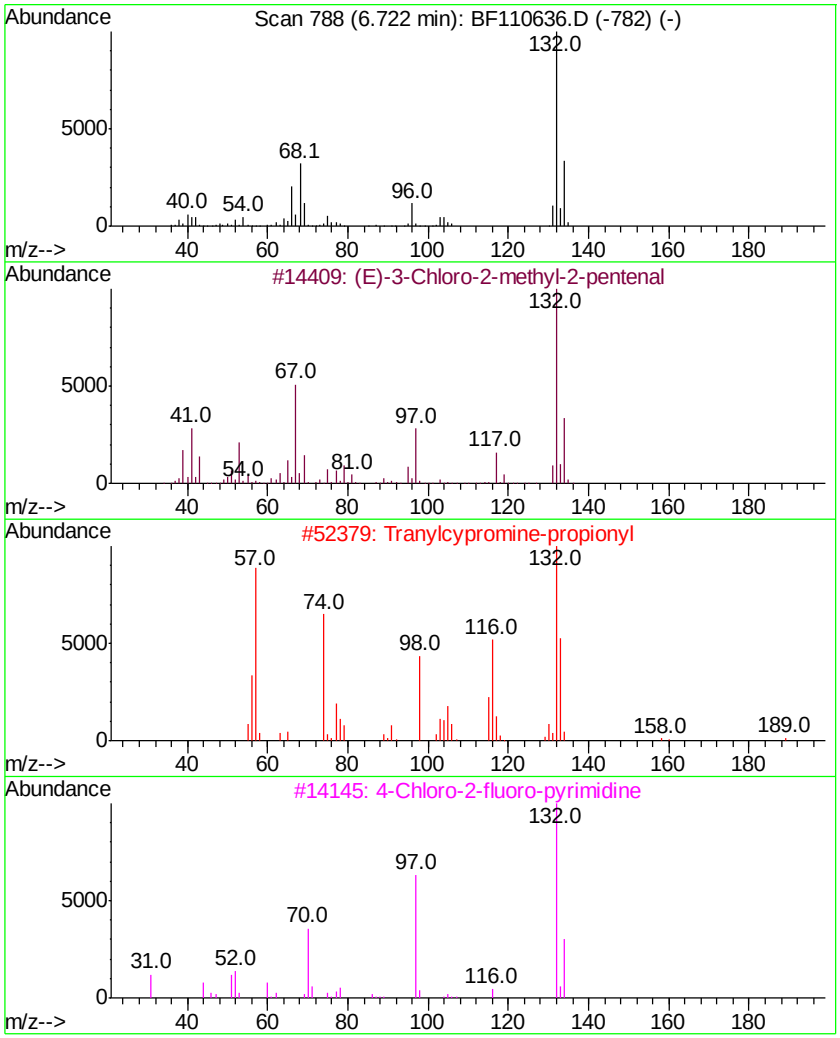
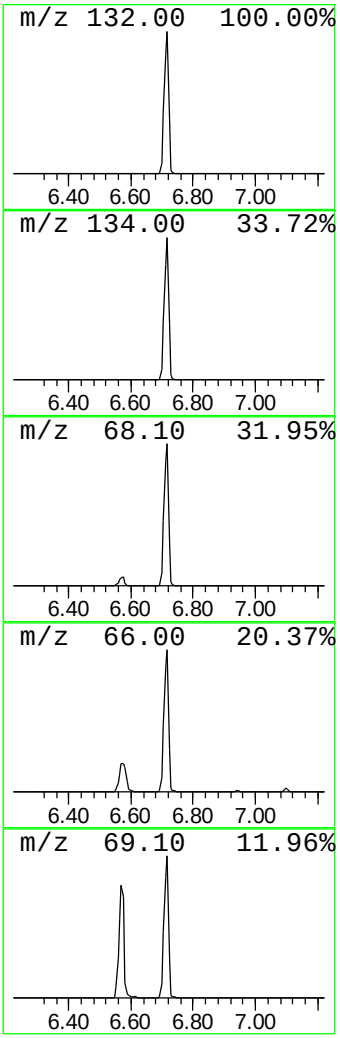
Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	100.25 ng	2237980	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





Library Search Compound Report

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Sample : J5864-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OLDMANS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

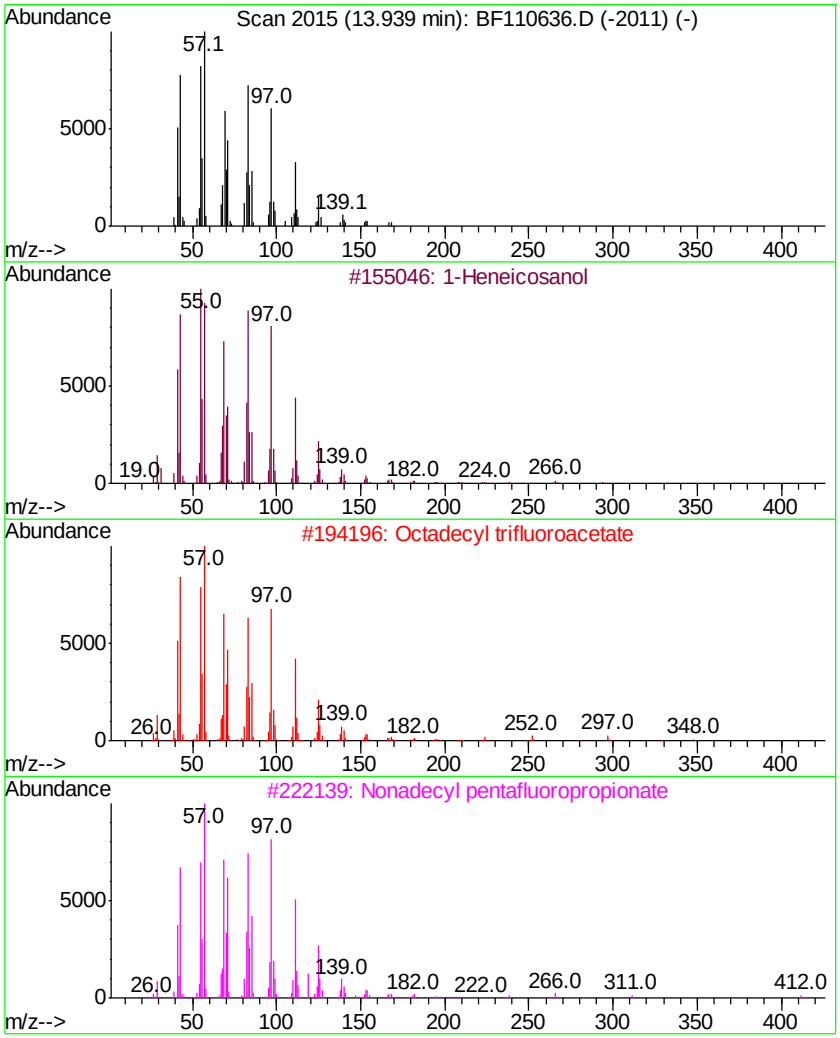
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

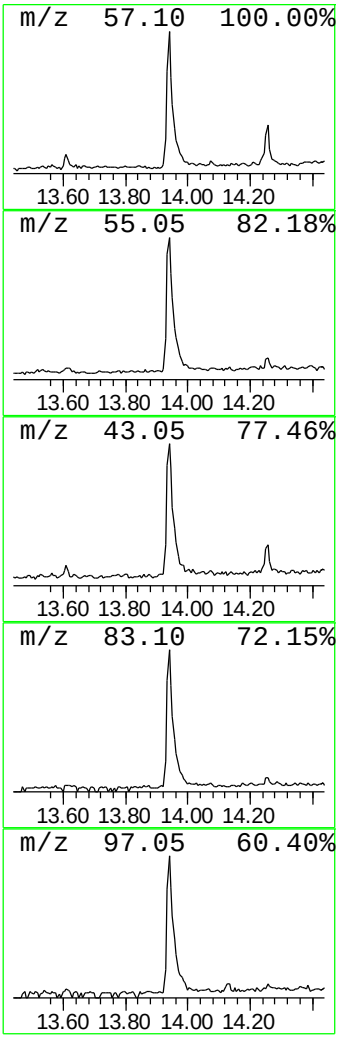
****

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	7.25 ng	244244	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	1-Docosene	308	C22H44	001599-67-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
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Operator : JU/SJ
Sample : J5864-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OLDMANS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

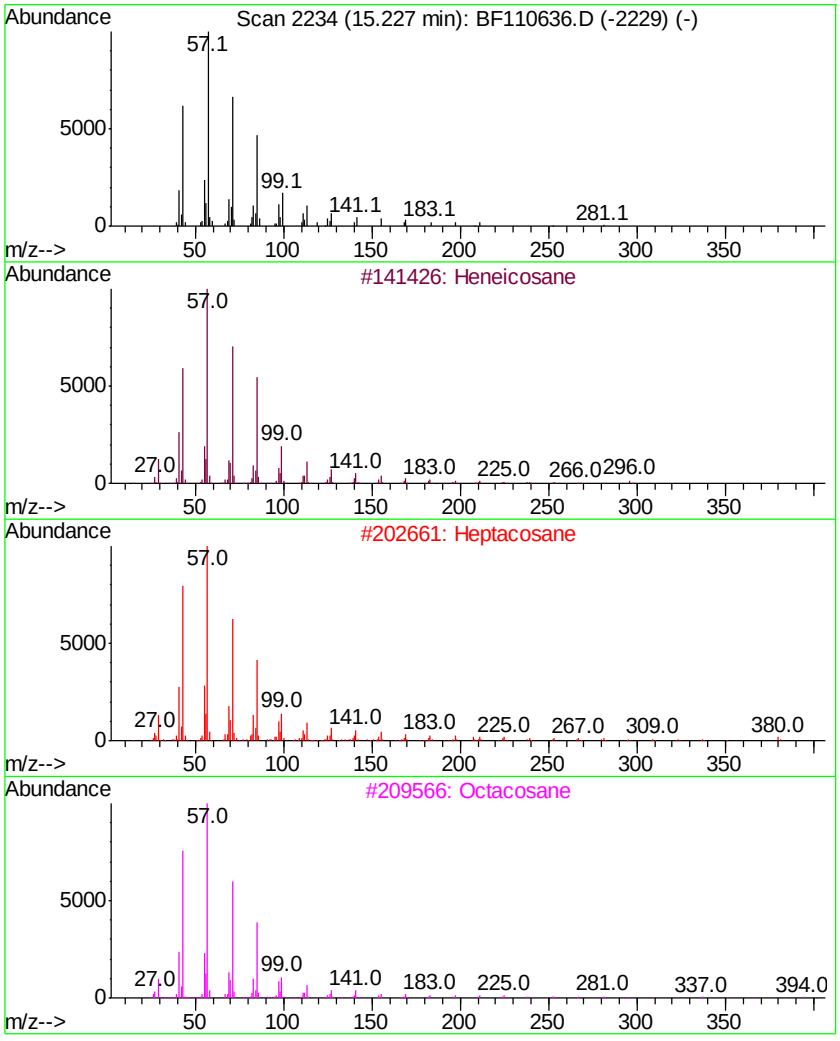
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

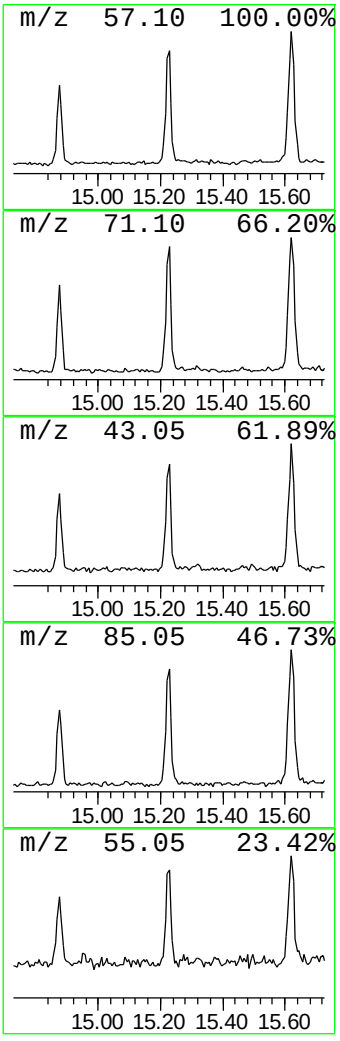
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	5.31 ng	103355	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Sample : J5864-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OLDMANS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

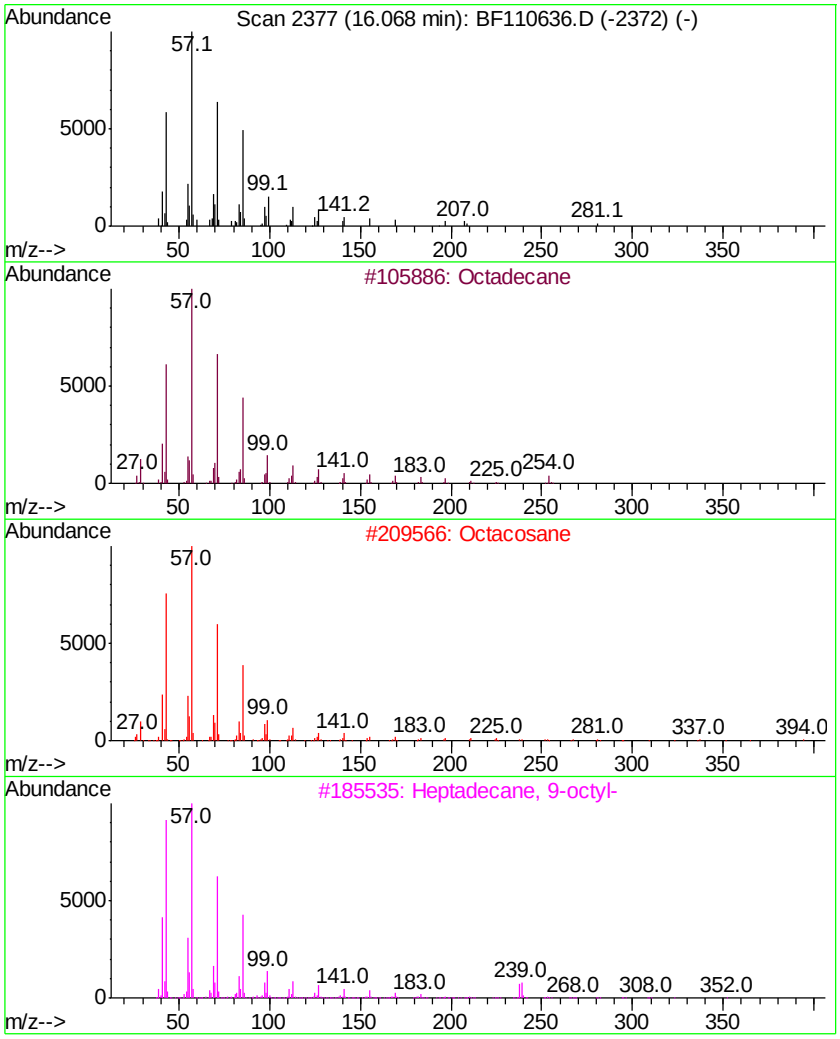
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

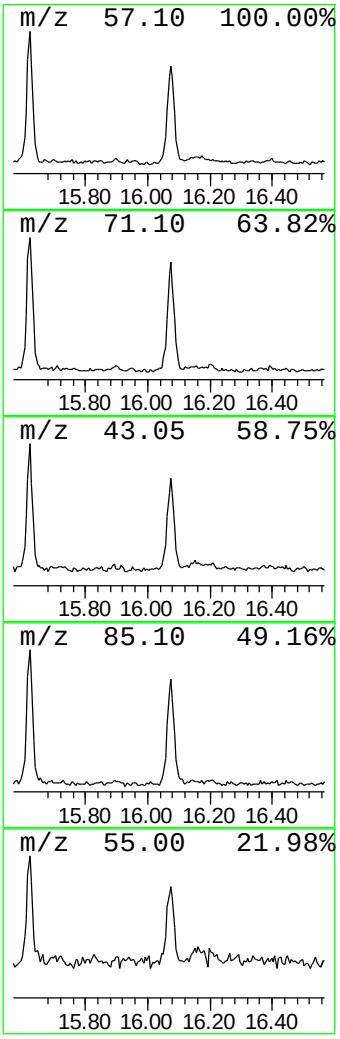
****

Peak Number 7 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	6.30 ng	122706	Perylene-d12	15.66

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	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Triacontane	422	C30H62	000638-68-6	91





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Sample : J5864-01
Misc :
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Instrument : BNA_F
ClientSampleId : OLDMANS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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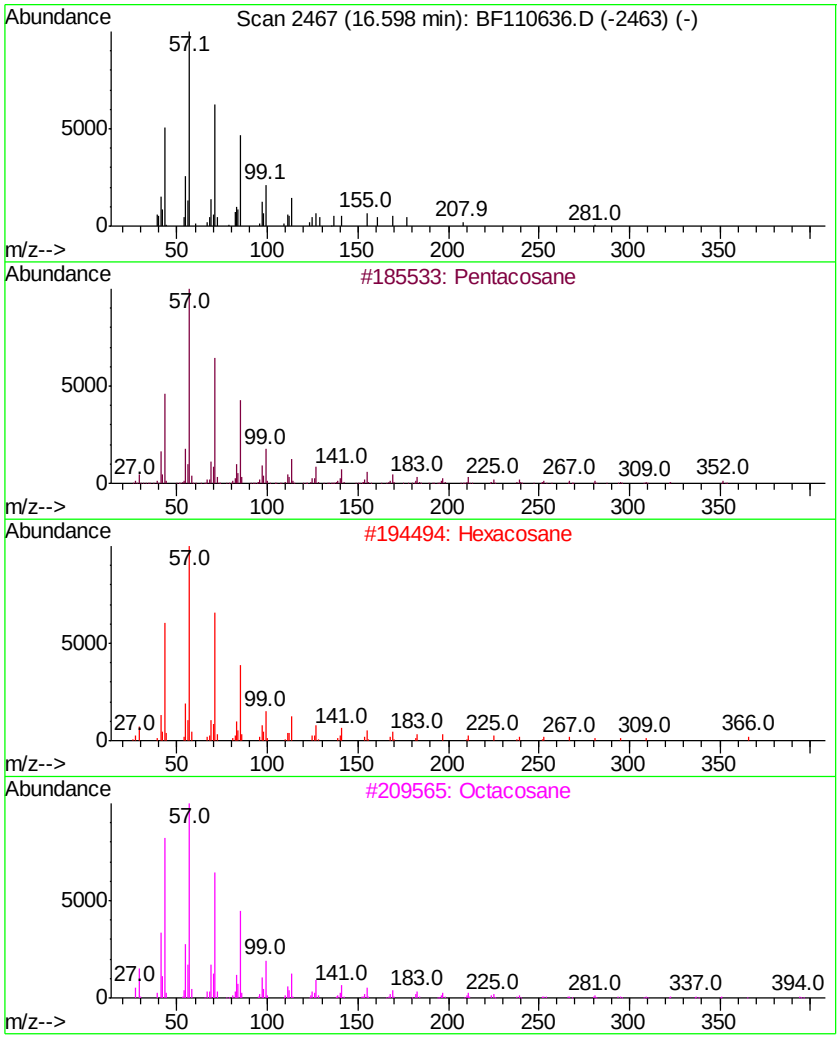
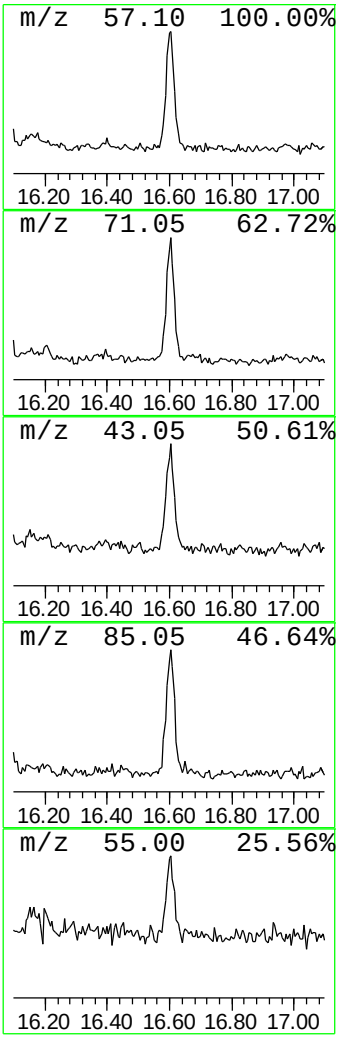
Peak Number 8 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	3.40 ng	66278	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Octacosane	394	C28H58	000630-02-4	86
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Heptadecane	240	C17H36	000629-78-7	83





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
Butane, 2-methoxy...	2.29	5.9	ng	132266	1	6.95	446484	20.0
2-Pentanone, 4-hy...	5.19	3.3	ng	73400	1	6.95	446484	20.0
unknown6.72	6.72	100.3	ng	2237980	1	6.95	446484	20.0
1-Heneicosanol	13.94	7.3	ng	244244	5	14.13	673851	20.0
Heneicosane	15.23	5.3	ng	103355	6	15.66	389646	20.0
Octadecane	16.07	6.3	ng	122706	6	15.66	389646	20.0
Pentacosane	16.60	3.4	ng	66278	6	15.66	389646	20.0