LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110726.D
Acq On : 13 Nov 2018 18:31
Operator : JU/SJ
Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-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:\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	2.275	28	32	42	rVB	106530	146527	7.25%	0.838%
2	5.186	523	527	540	rBV	58010	89957	4.45%	0.514%
3	5.569	587	592	607	rBV	1859916	1844697	91.31%	10.548%
4	6.569	758	762	782	rBV	1793193	2020173	100.00%	11.551%
5	6.716	782	787	790	rBV	2078162	1967165	97.38%	11.248%
6	6.945	822	826	832	rBV	499202	458733	22.71%	2.623%
7	7.098	848	852	868	rBV	1692879	1485326	73.52%	8.493%
8	7.510	917	922	939	rBV	1253887	1244761	61.62%	7.117%
9	8.227	1040	1044	1059	rBV	550053	600263	29.71%	3.432%
10	9.298	1222	1226	1229	rBV	2429457	1997752	98.89%	11.423%
11	9.692	1287	1293	1300	rBV	89059	86640	4.29%	0.495%
12	9.986	1339	1343	1349	rBV	637569	624292	30.90%	3.570%
13	10.774	1473	1477	1488	rBV	1063532	1101408	54.52%	6.298%
14	11.480	1593	1597	1606	rBV	540414	521721	25.83%	2.983%
15	11.980	1678	1682	1691	rBV2	50446	60040	2.97%	0.343%
16	13.057	1861	1865	1869	rBV	1372914	1281476	63.43%	7.327%
17	13.933	2011	2014	2026	rVB	76956	94826	4.69%	0.542%
18	14.127	2043	2047	2054	rBV	407120	402187	19.91%	2.300%
19	14.251	2065	2068	2074	rVB	25065	27205	1.35%	0.156%
20	14.556	2116	2120	2125	rBV	54599	66294	3.28%	0.379%
21	14.874	2170	2174	2180	rVB	91809	94883	4.70%	0.543%
22	15.221	2229	2233	2239	rVB	140963	162885	8.06%	0.931%
23	15.615	2295	2300	2303	rBV	173064	231467	11.46%	1.323%
24	15.656	2303	2307	2317	rVB	287086	395818	19.59%	2.263%
25	16.068	2371	2377	2384	rBV	147727	238869	11.82%	1.366%
26	16.598	2461	2467	2475	rBV	80491	146593	7.26%	0.838%
27	17.221	2566	2573	2580	rVB2	28997	62335	3.09%	0.356%
28	17.950	2690	2697	2705	rVB5	13202	34801	1.72%	0.199%

Sum of corrected areas: 17489094

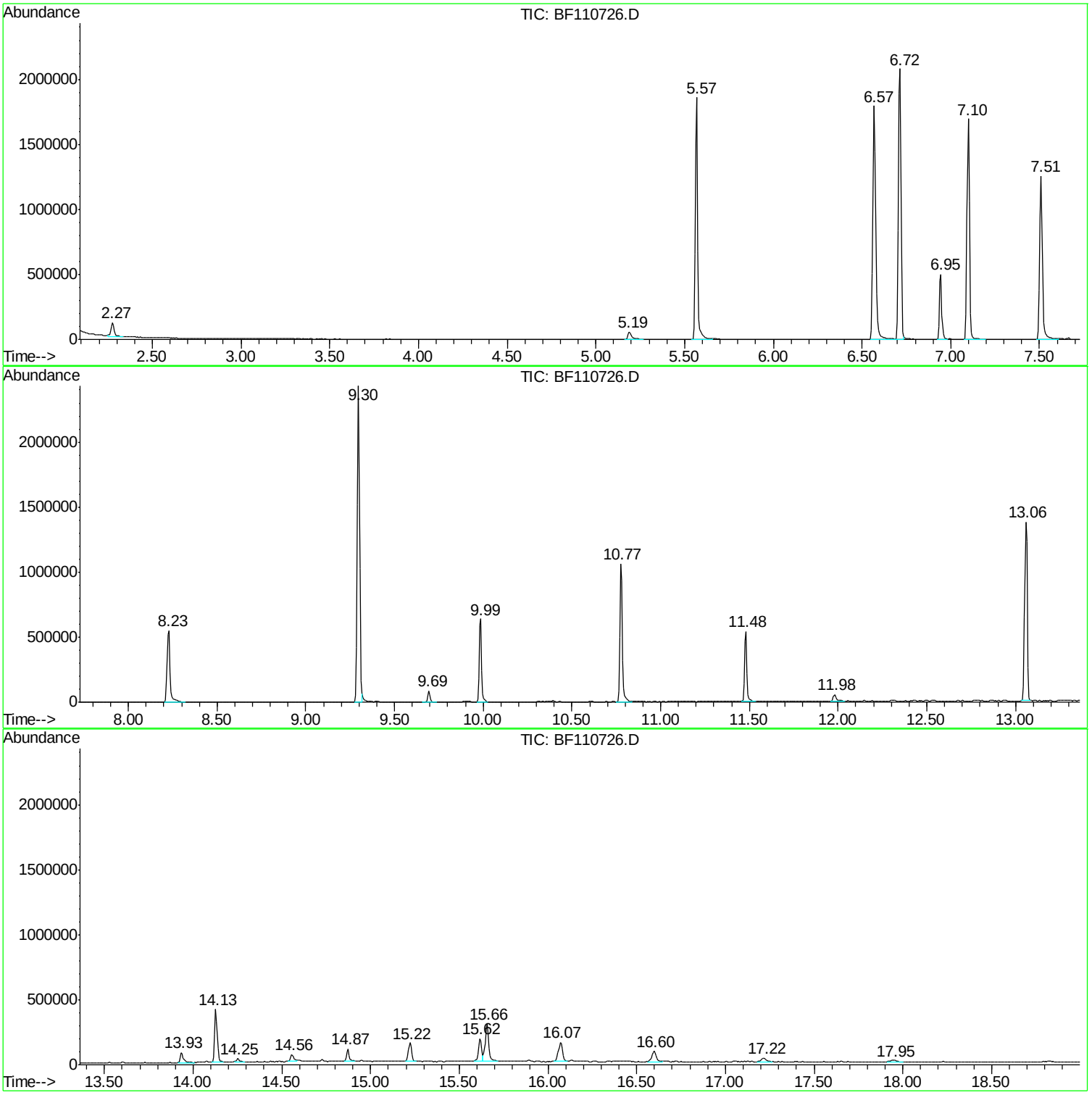
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110726.D
Acq On : 13 Nov 2018 18:31
Operator : JU/SJ
Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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\BF111318\
Data File : BF110726.D
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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

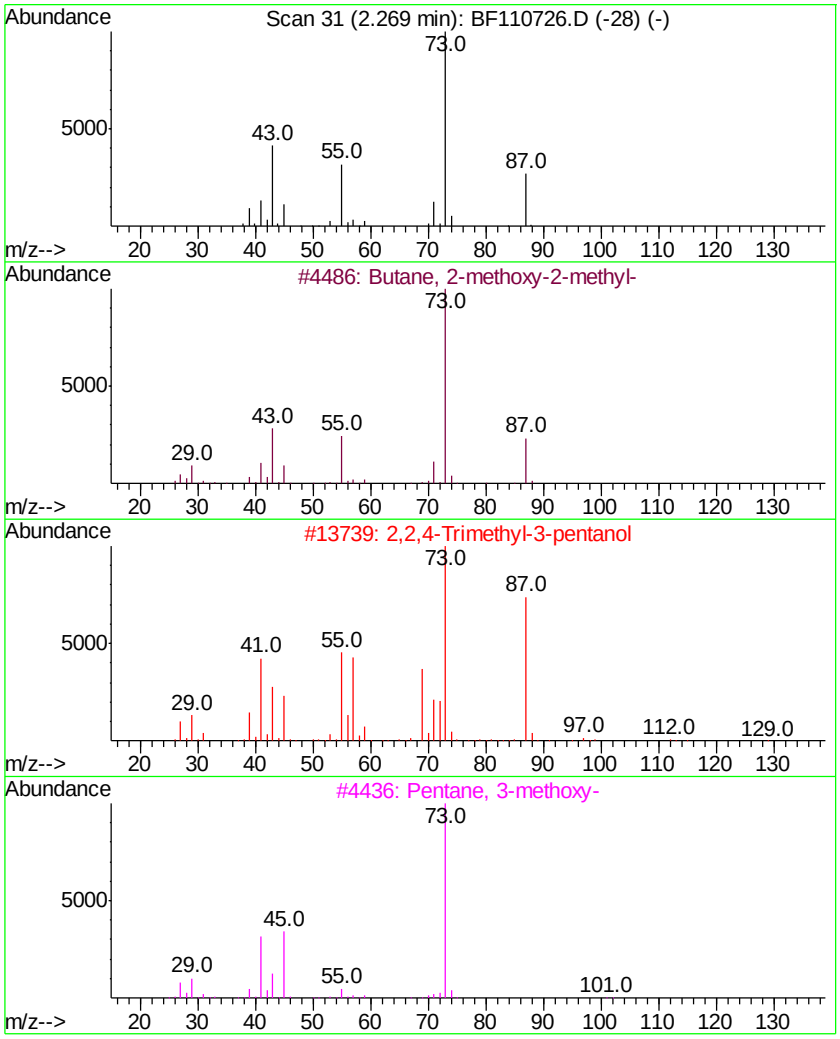
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

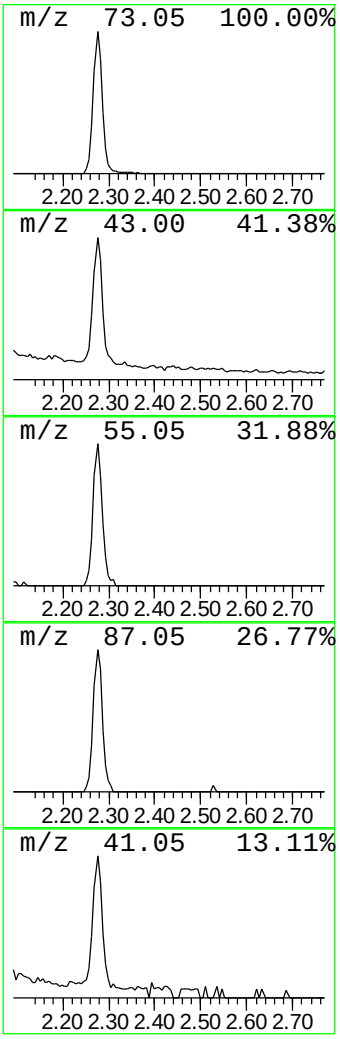
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	6.39 ng	146527	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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Library Search Compound Report

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Operator : JU/SJ
Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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

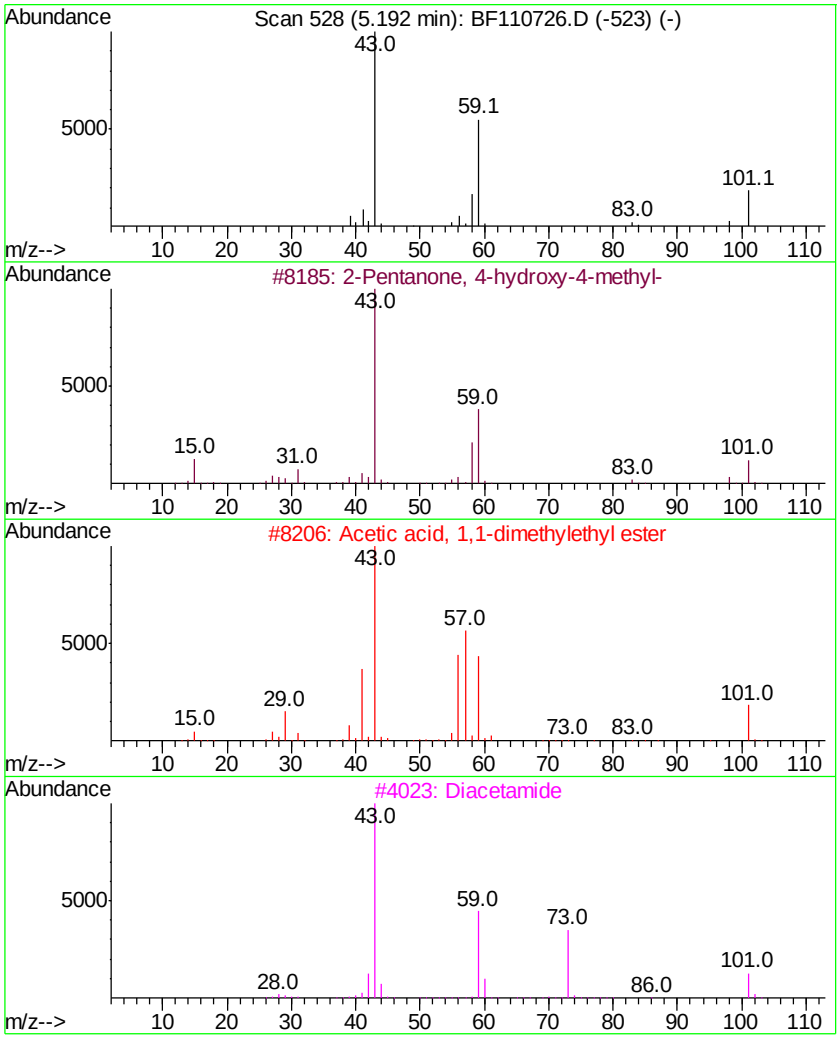
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

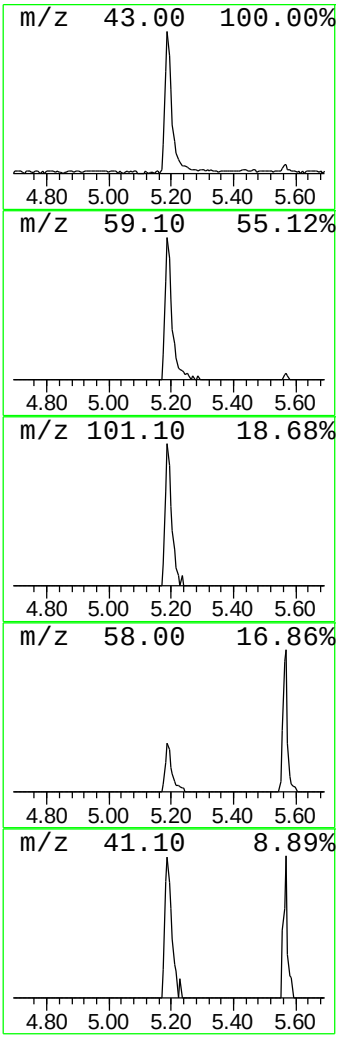
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.92 ng	89957	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9





Library Search Compound Report

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Data File : BF110726.D
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Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
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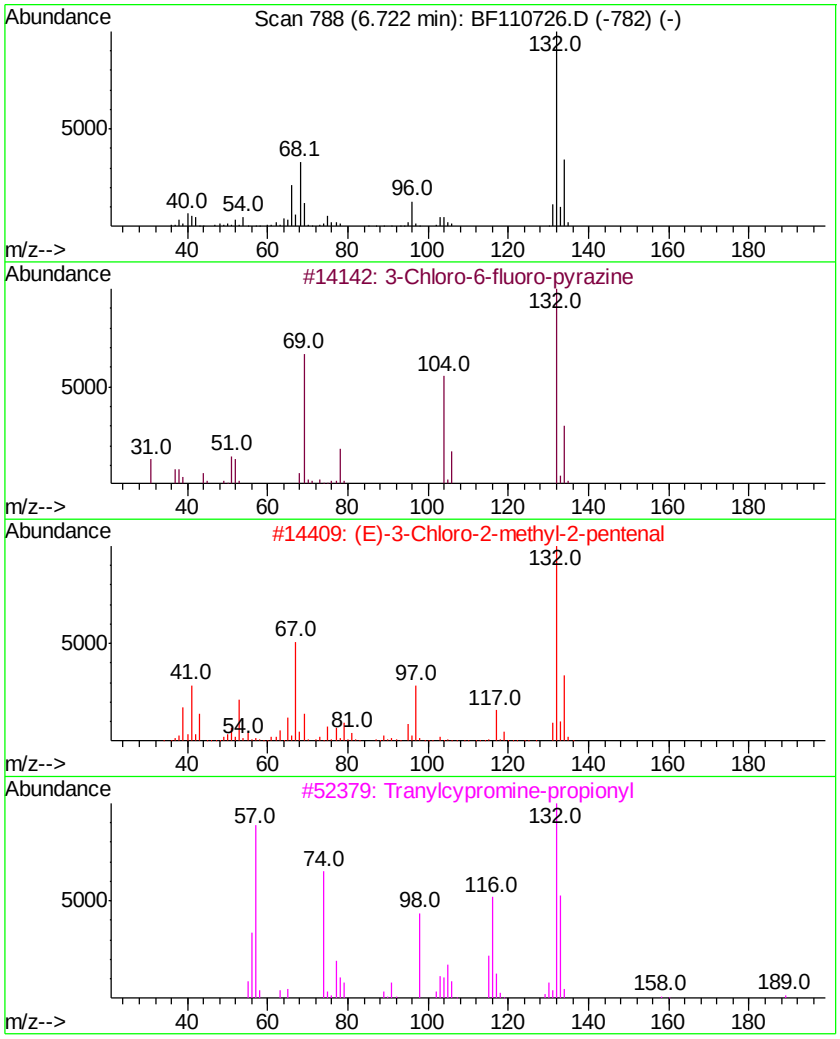
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

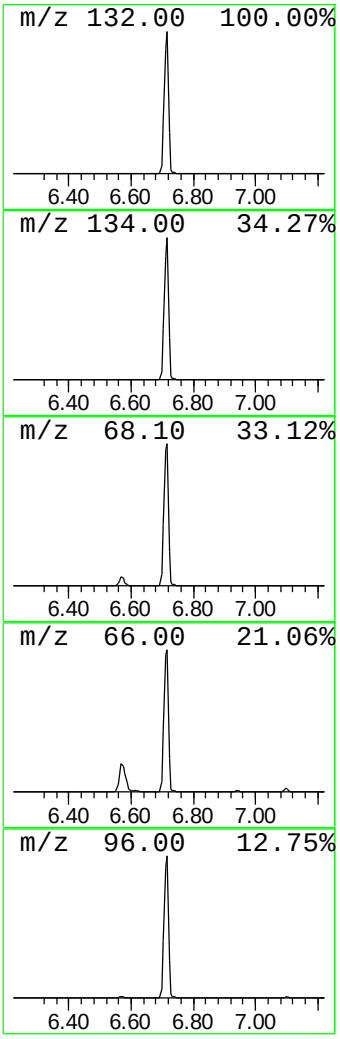
****

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	85.77 ng	1967170	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Data File : BF110726.D
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Operator : JU/SJ
Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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

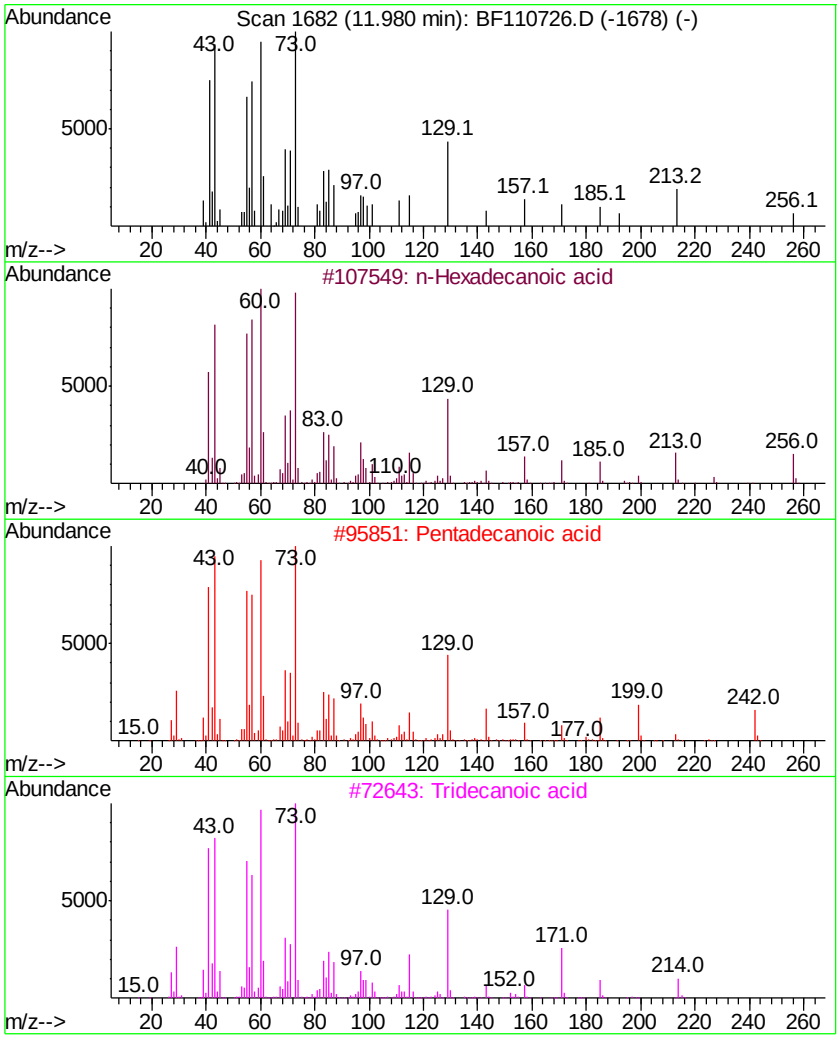
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

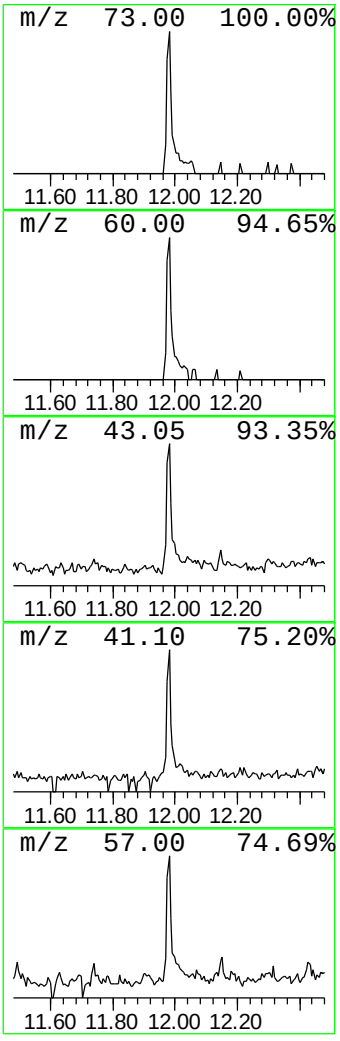
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	2.30 ng	60040	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
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Operator : JU/SJ
Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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

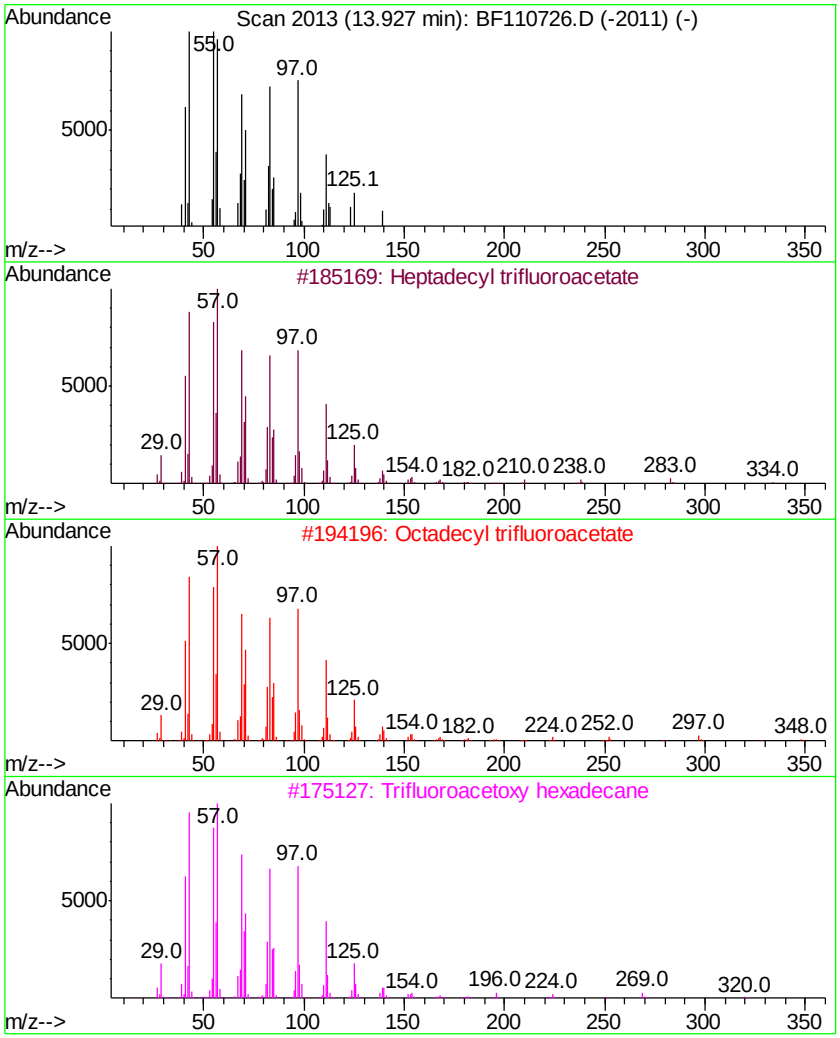
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

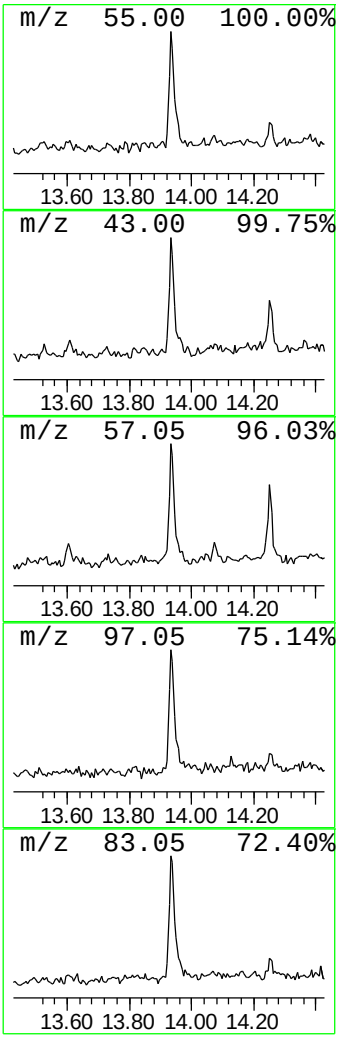
****

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	4.72 ng	94826	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
5	Octacosanol	410	C28H58O	000557-61-9	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
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Operator : JU/SJ
Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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

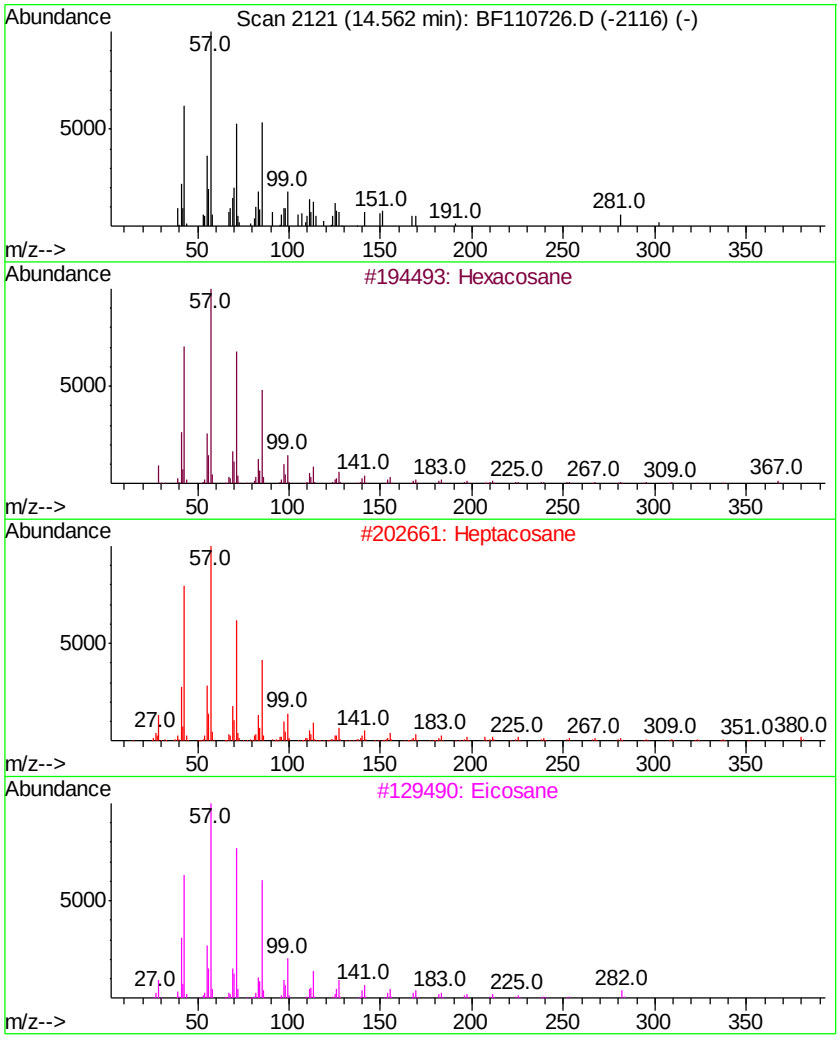
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

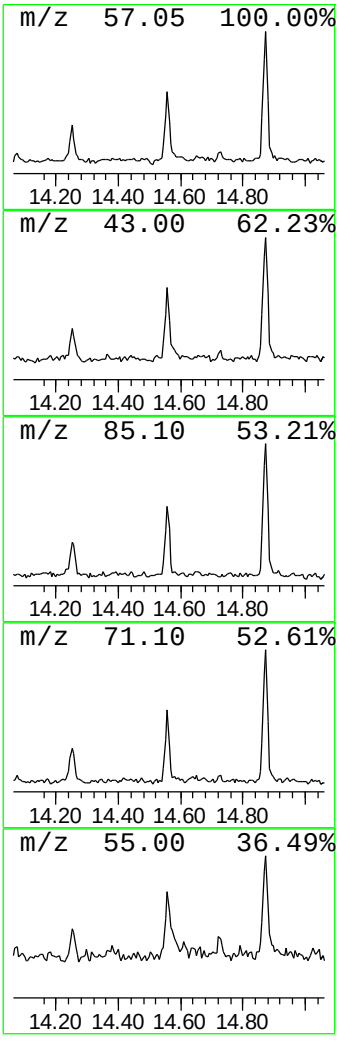
****

Peak Number 7 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	3.30 ng	66294	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Octacosane	394	C28H58	000630-02-4	90





Library Search Compound Report

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Data File : BF110726.D
Acq On : 13 Nov 2018 18:31
Operator : JU/SJ
Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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

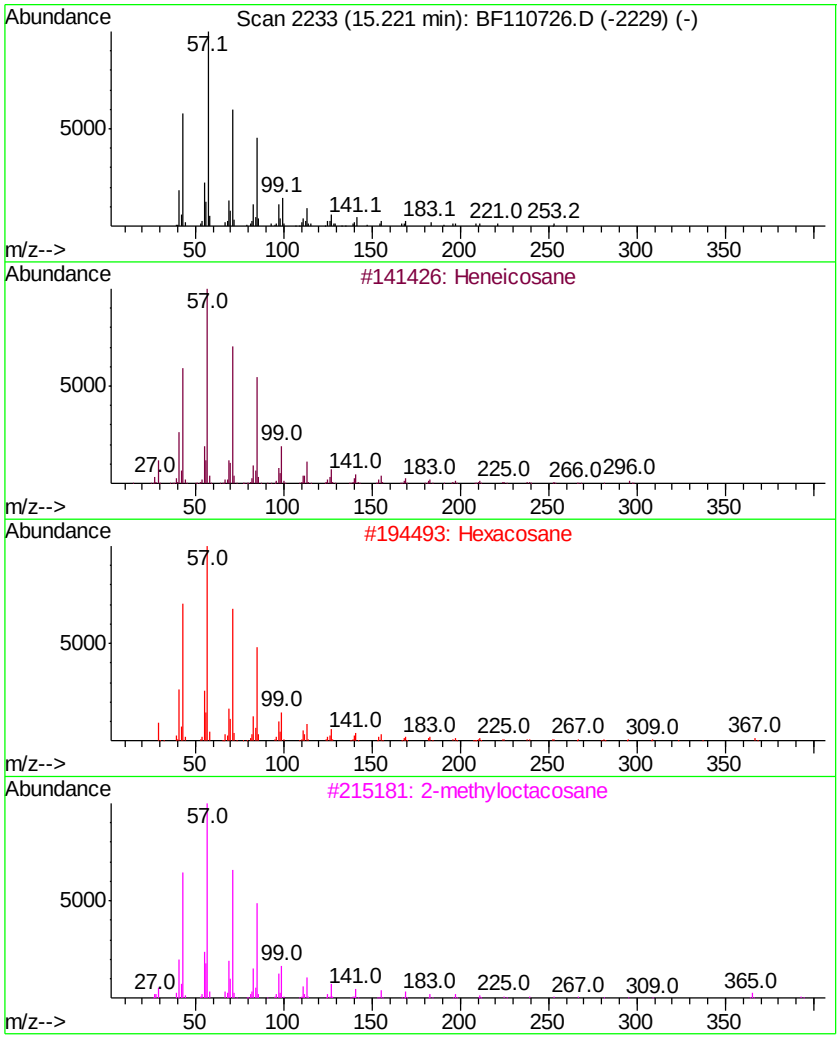
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

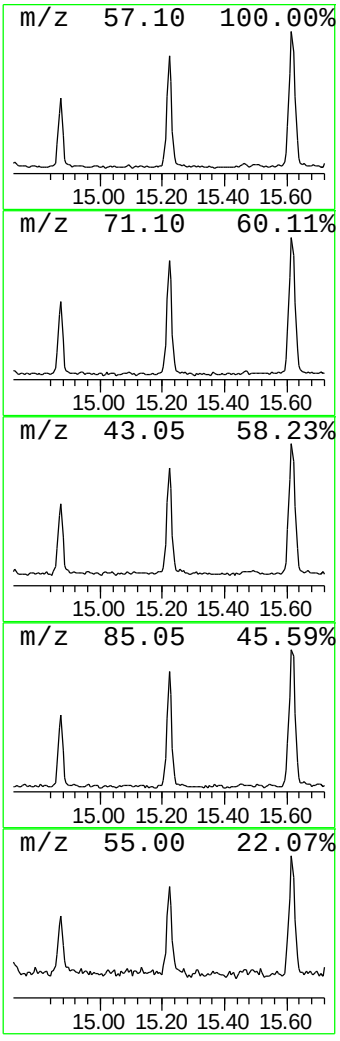
****

Peak Number 9 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	8.23 ng	162885	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Heptacosane	380	C27H56	000593-49-7	87





Library Search Compound Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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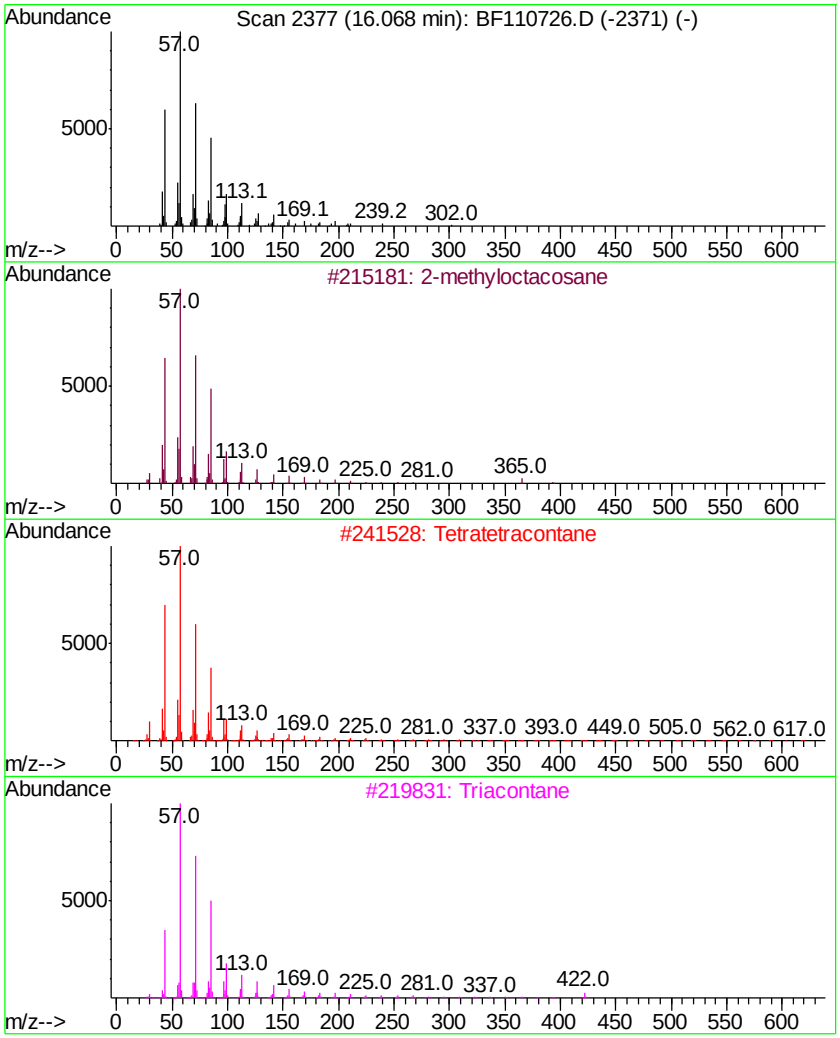
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

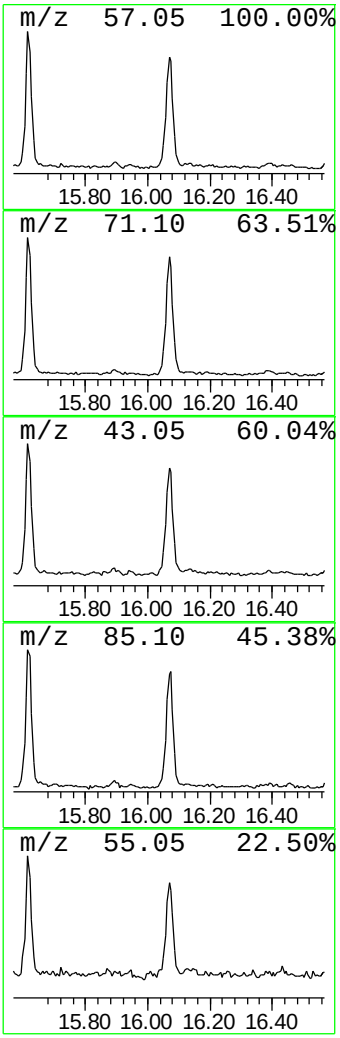
****

Peak Number 10 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	12.07 ng	238869	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Sample : J5909-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-S

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

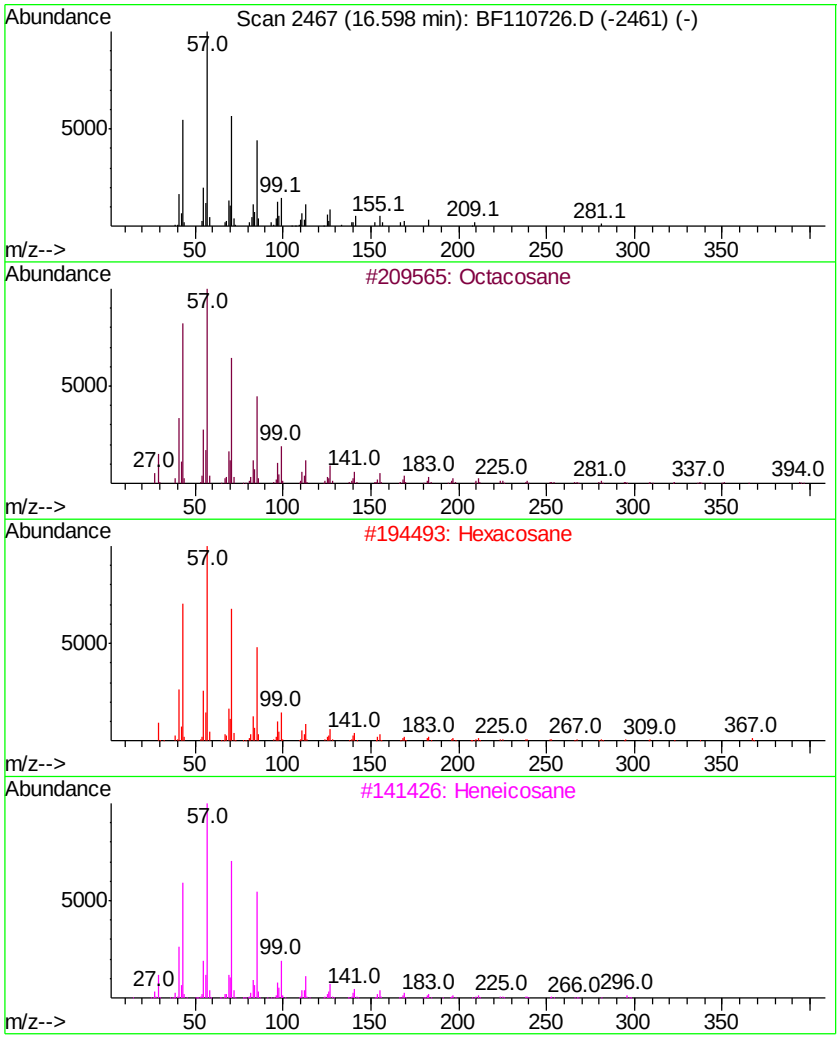
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

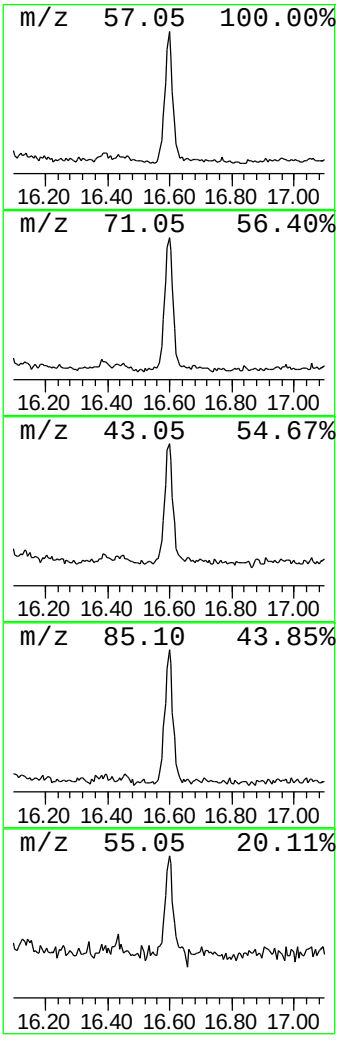
****

Peak Number 11 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	7.41 ng	146593	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexatriacontane	507	C36H74	000630-06-8	91
5	Hentriacontane	437	C31H64	000630-04-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111318\
Data File : BF110726.D
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Operator : JU/SJ
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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...	2.27	6.4	ng	146527	1	6.95	458733	20.0
2-Pentanone, 4-hy...	5.19	3.9	ng	89957	1	6.95	458733	20.0
unknown6.72	6.72	85.8	ng	1967170	1	6.95	458733	20.0
n-Hexadecanoic acid	11.98	2.3	ng	60040	4	11.48	521721	20.0
Heptadecyl triflu...	13.93	4.7	ng	94826	5	14.13	402187	20.0
Hexacosane	14.56	3.3	ng	66294	5	14.13	402187	20.0
Heneicosane	15.22	8.2	ng	162885	6	15.66	395818	20.0
2-methyloctacosane	16.07	12.1	ng	238869	6	15.66	395818	20.0
Octacosane	16.60	7.4	ng	146593	6	15.66	395818	20.0