LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110647.D
Acq On : 10 Nov 2018 00:20
Operator : JU/SJ
Sample : J5884-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8A-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	2.269	26	31	50	rVB	112404	177925	8.35%	1.042%
2	5.193	524	528	543	rBV	48329	75626	3.55%	0.443%
3	5.569	588	592	595	rBV	2007243	1874704	88.00%	10.979%
4	6.575	757	763	772	rBV	1897438	2130285	100.00%	12.476%
5	6.716	783	787	790	rBV	2290613	2031833	95.38%	11.899%
6	6.945	822	826	832	rBV	576666	483345	22.69%	2.831%
7	7.098	848	852	865	rBV	1554530	1461081	68.59%	8.557%
8	7.510	917	922	925	rBV	1305613	1215766	57.07%	7.120%
9	8.228	1040	1044	1056	rBV	680568	626517	29.41%	3.669%
10	9.298	1222	1226	1235	rBV	2188315	1897893	89.09%	11.115%
11	9.692	1287	1293	1300	rBV	93759	86450	4.06%	0.506%
12	9.986	1339	1343	1350	rBV	720825	623127	29.25%	3.649%
13	10.780	1474	1478	1490	rBV	992778	962043	45.16%	5.634%
14	11.480	1593	1597	1605	rBV	574286	524679	24.63%	3.073%
15	11.980	1680	1682	1686	rBV2	66282	62390	2.93%	0.365%
16	12.698	1801	1804	1810	rBV	23883	22475	1.06%	0.132%
17	12.933	1841	1844	1848	rVB	26276	23676	1.11%	0.139%
18	13.063	1862	1866	1869	rBV	1652160	1383591	64.95%	8.103%
19	13.257	1892	1899	1907	rBV5	13491	31115	1.46%	0.182%
20	13.939	2011	2015	2021	rBV	176609	227584	10.68%	1.333%
21	14.127	2043	2047	2051	rBV	466790	466074	21.88%	2.730%
22	14.563	2117	2121	2129	rBV2	79383	141124	6.62%	0.826%
23	14.874	2171	2174	2178	rVB	31564	35023	1.64%	0.205%
24	15.227	2231	2234	2238	rVB	90639	98031	4.60%	0.574%
25	15.621	2298	2301	2303	rBV3	29916	37381	1.75%	0.219%
26	15.657	2303	2307	2312	rVB	250400	314842	14.78%	1.844%
27	16.074	2375	2378	2384	rVB	42093	60490	2.84%	0.354%

Sum of corrected areas: 17075070

LSC Report - Integrated Chromatogram

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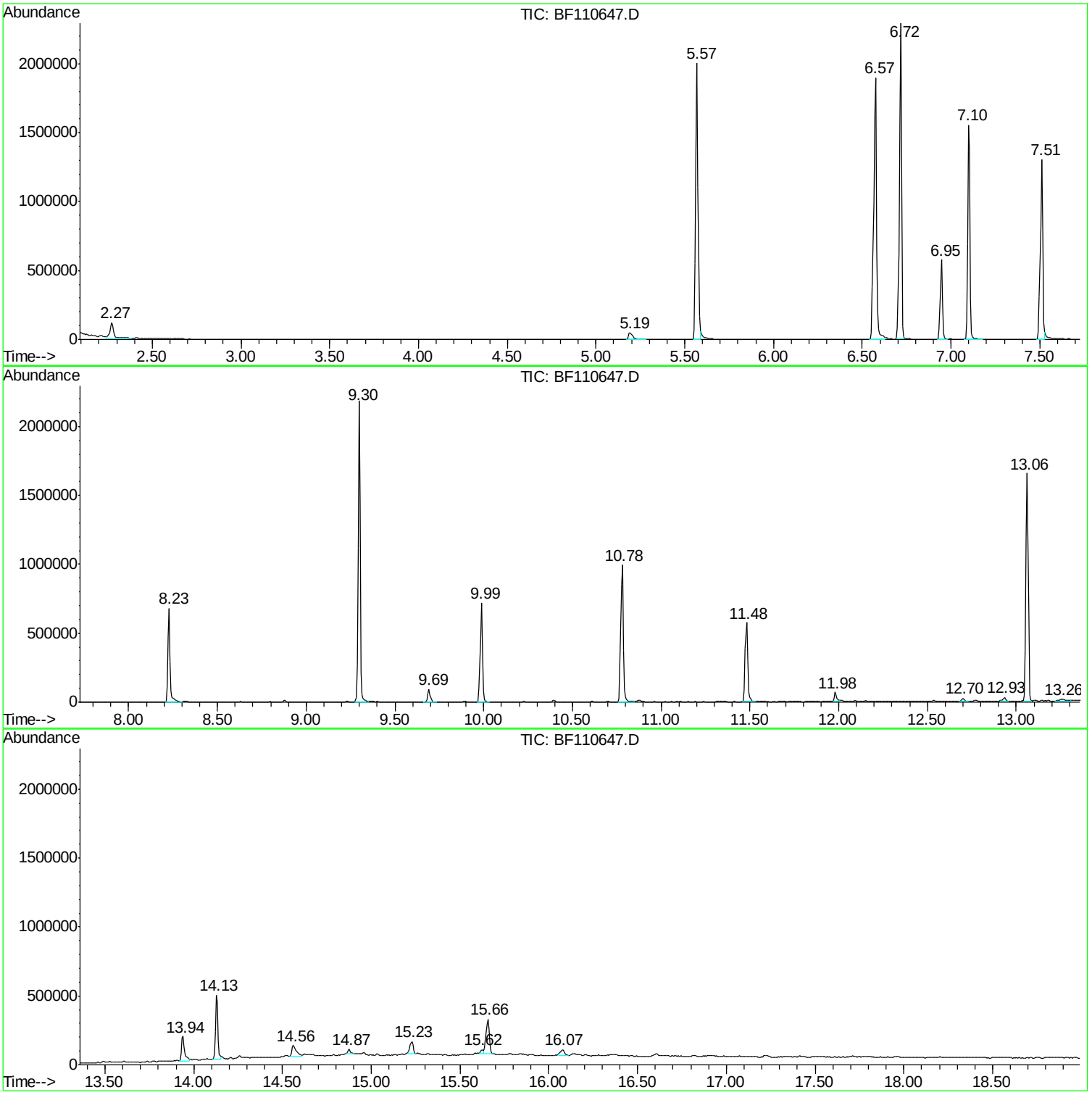
Sample : J5884-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8A-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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

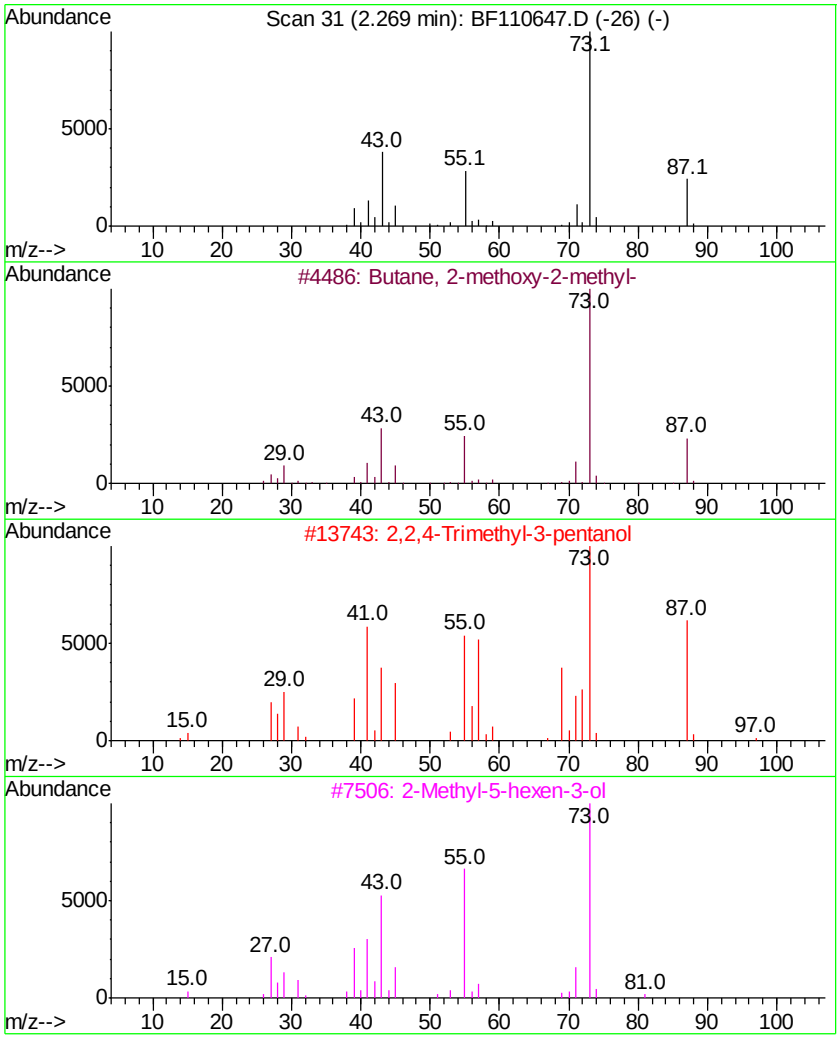
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

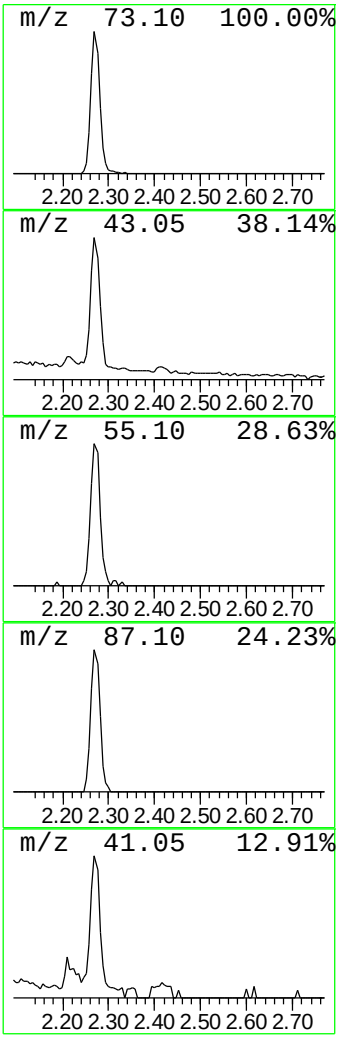
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	7.36 ng	177925	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	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12





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Sample : J5884-11
Misc :
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Instrument : BNA_F
ClientSampleId : TP-8A-S

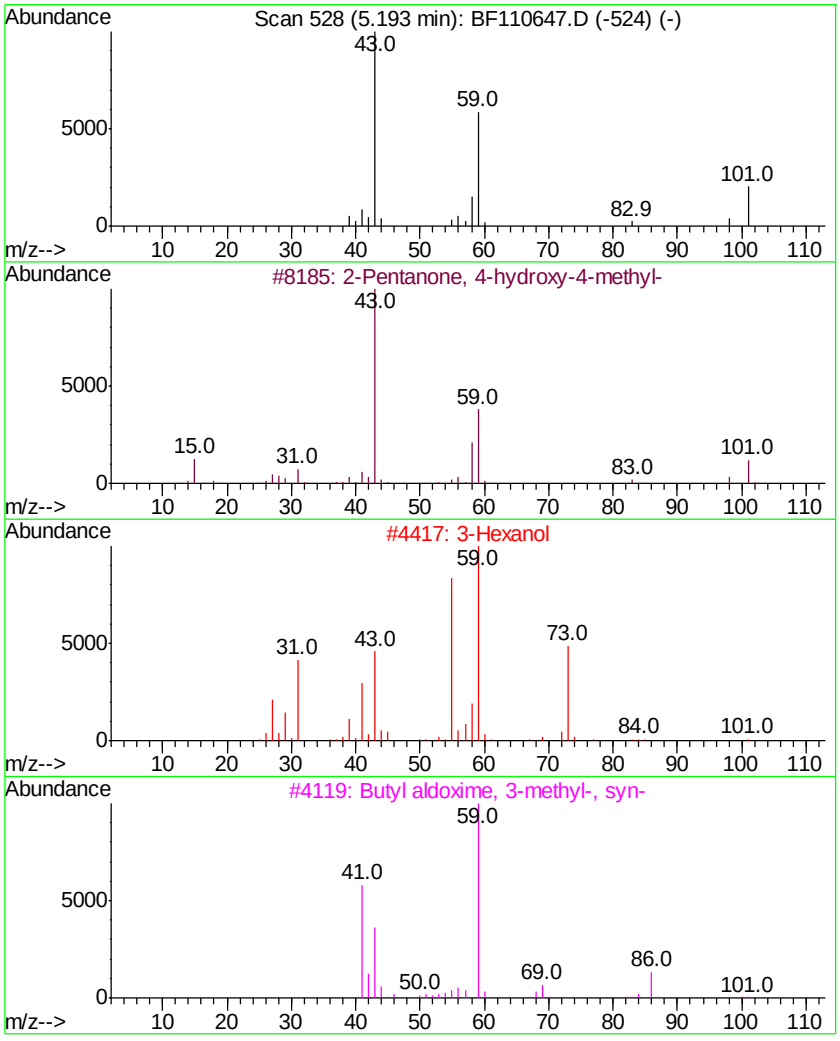
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

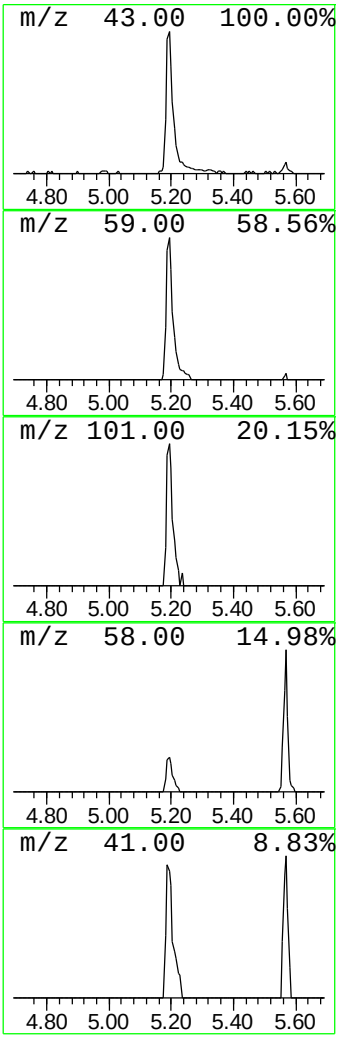
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.13 ng	75626	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	3-Hexanol	102	C6H14O	000623-37-0	28
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4	Propylamine	59	C3H9N	000107-10-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

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Sample : J5884-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8A-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

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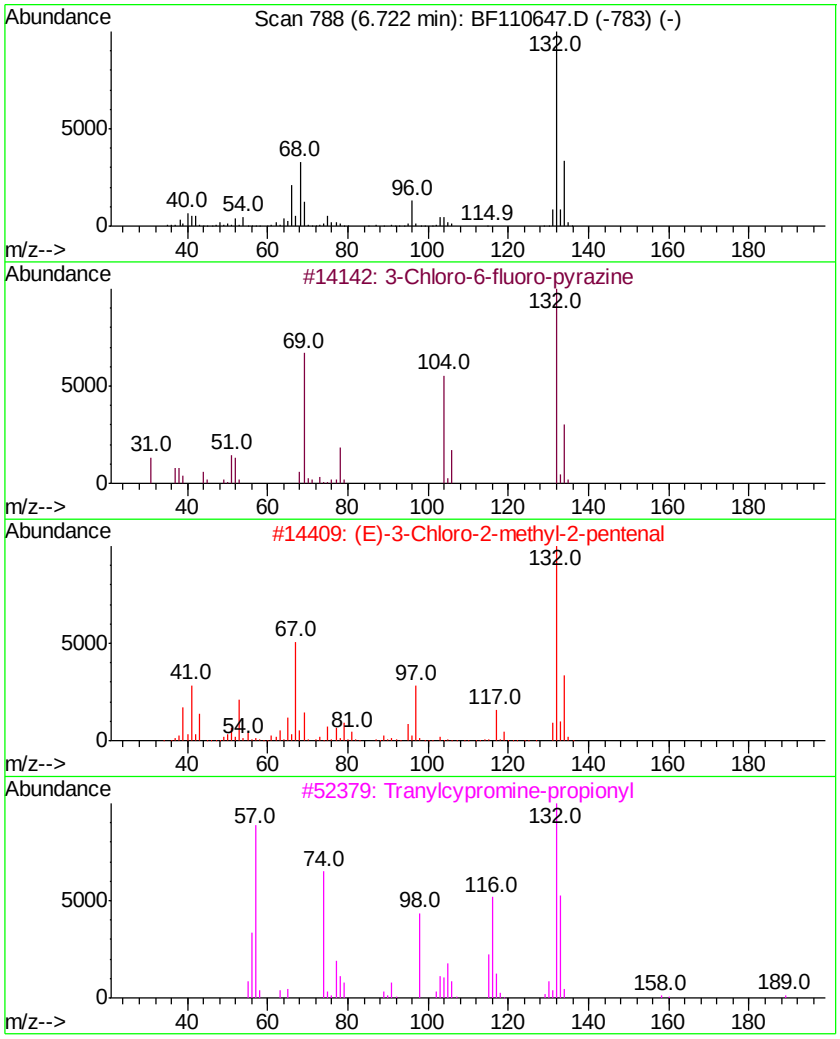
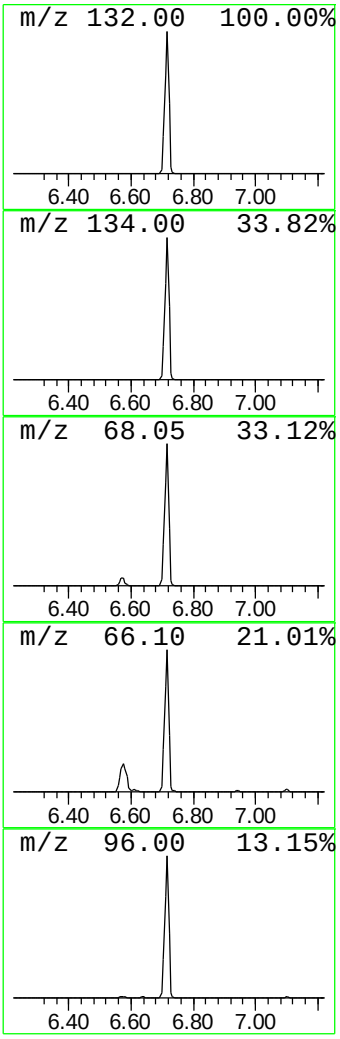
Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	84.07 ng	2031830	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	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TP-8A-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
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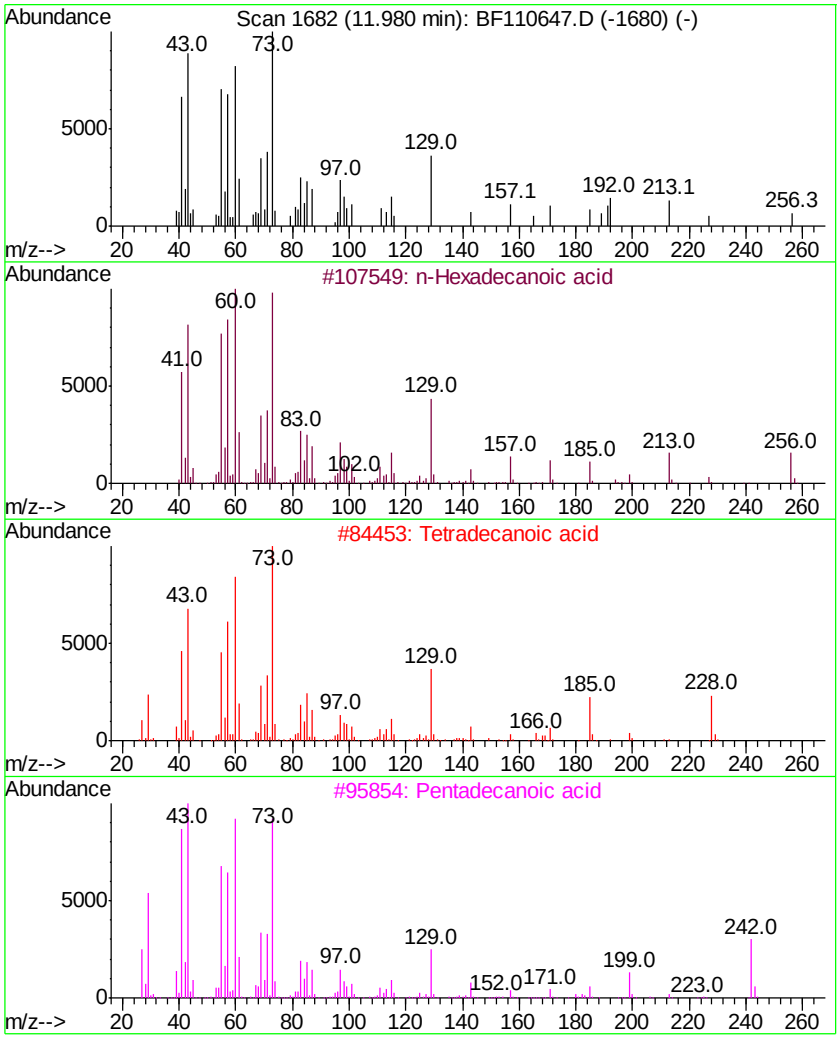
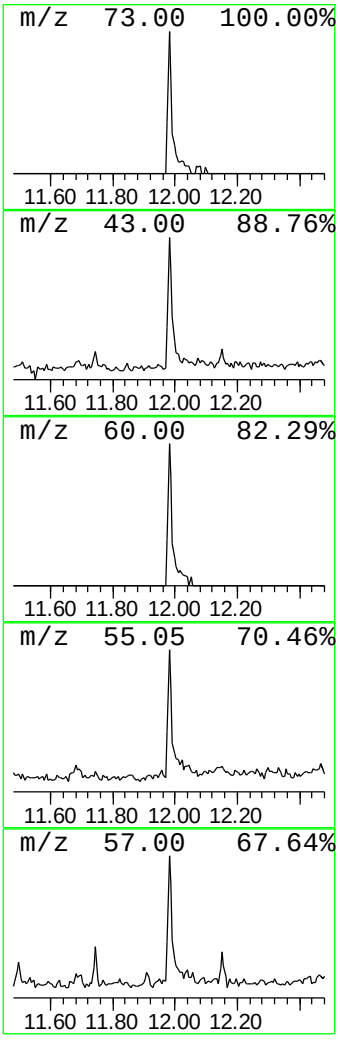
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	2.38 ng	62390	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
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Sample : J5884-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8A-S

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

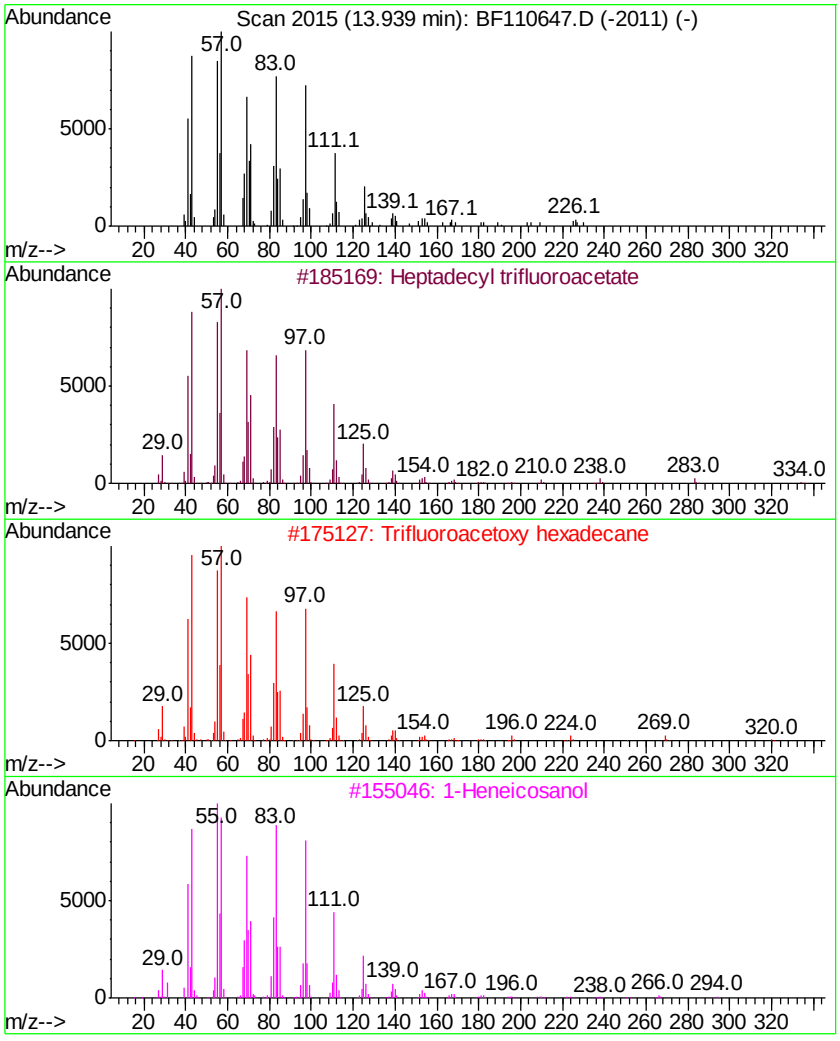
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

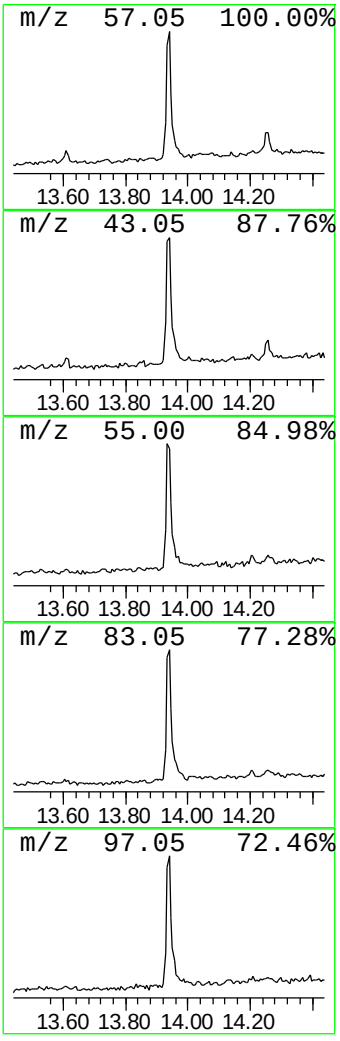
****

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	9.77 ng	227584	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95





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Instrument : BNA_F
ClientSampleId : TP-8A-S

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

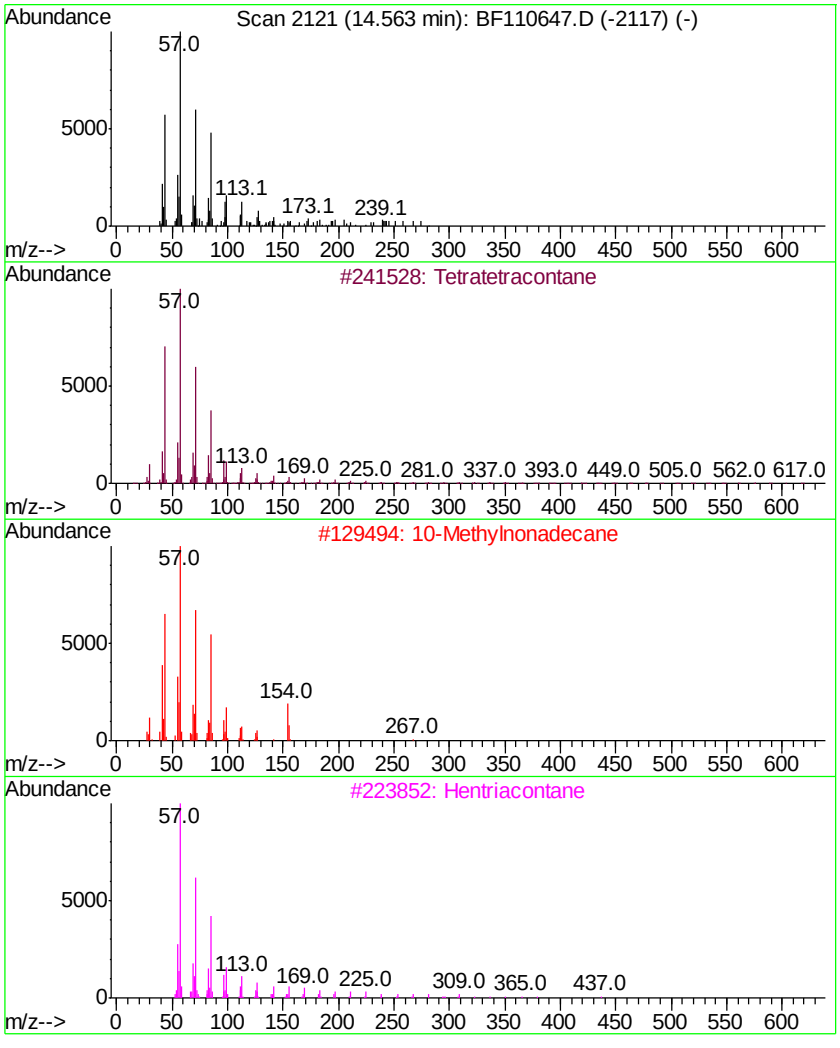
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

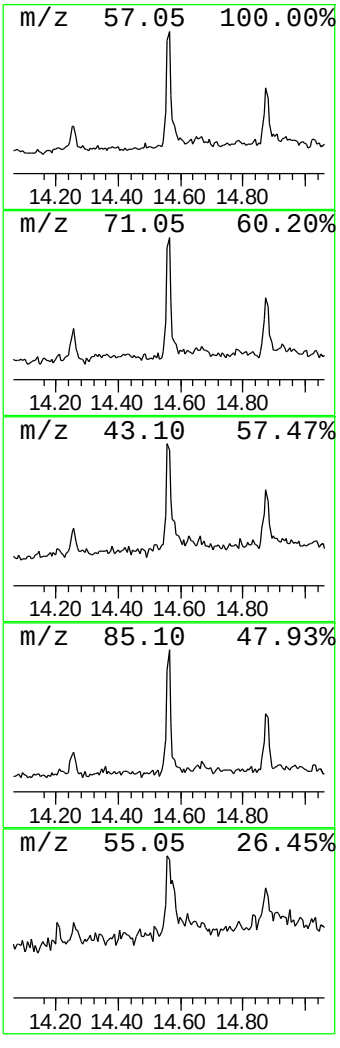
****

Peak Number 7 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	6.06 ng	141124	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	10-Methylnonadecane	282	C20H42	056862-62-5	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octacosane	394	C28H58	000630-02-4	90





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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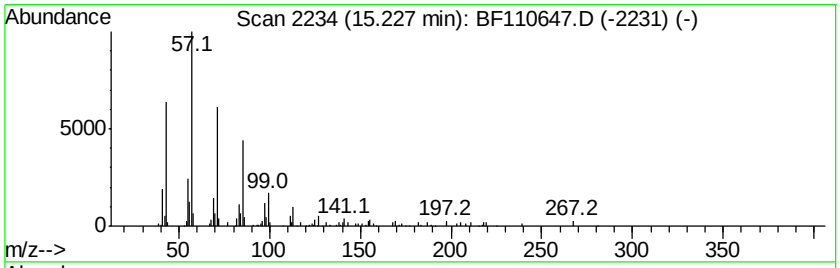
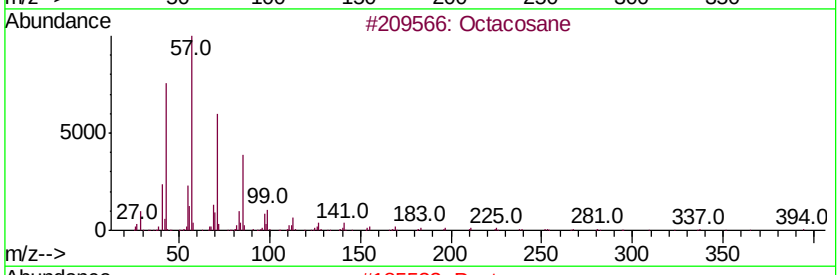
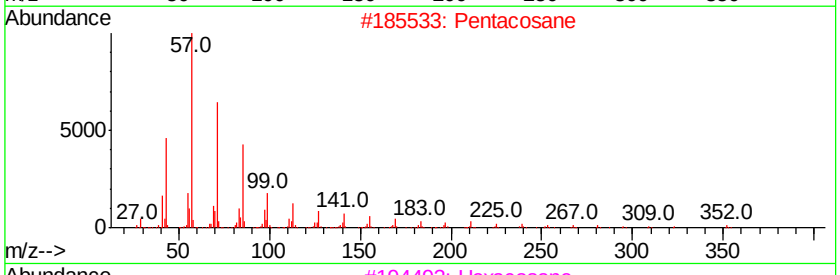
Peak Number 8 Octacosane Concentration Rank 5

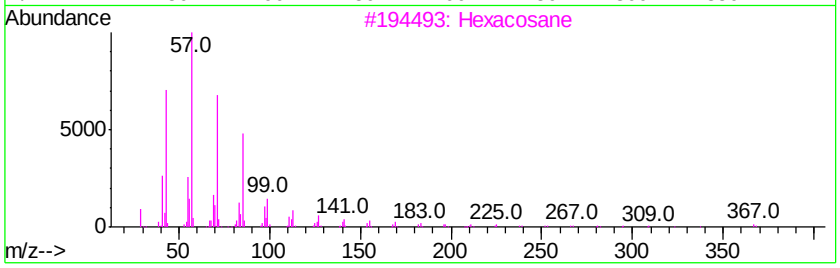
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	6.23 ng	98031	Perylene-d12	15.66

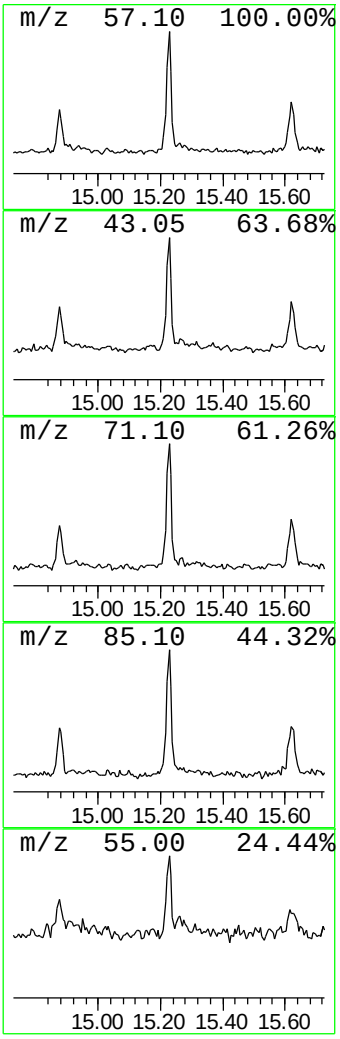
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90











Tentatively Identified Compound (LSC) summary

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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	7.4	ng	177925	1	6.95	483345	20.0
2-Pentanone, 4-hy...	5.19	3.1	ng	75626	1	6.95	483345	20.0
unknown6.72	6.72	84.1	ng	2031830	1	6.95	483345	20.0
n-Hexadecanoic acid	11.98	2.4	ng	62390	4	11.48	524679	20.0
Heptadecyl triflu...	13.94	9.8	ng	227584	5	14.13	466074	20.0
Tetratetracontane	14.56	6.1	ng	141124	5	14.13	466074	20.0
Octacosane	15.23	6.2	ng	98031	6	15.66	314842	20.0