LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050219\
Data File : BF114088.D
Acq On : 2 May 2019 16:58
Operator : JU/SJ
Sample : K2652-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-4

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-BF042219.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	2.128	3	7	15	rVB	29818	45815	1.95%	0.264%
2	5.510	578	582	597	rBV	1761493	1816514	77.39%	10.468%
3	6.522	749	754	768	rBV	1785916	1667613	71.05%	9.610%
4	6.657	773	777	781	rBV	1811592	1668670	71.09%	9.616%
5	6.886	813	816	820	rBV	500593	392250	16.71%	2.260%
6	7.045	839	843	846	rBV	1706151	1393556	59.37%	8.030%
7	7.445	907	911	924	rBV	1144438	1015297	43.26%	5.851%
8	8.169	1030	1034	1051	rBV	621679	601946	25.65%	3.469%
9	9.245	1213	1217	1229	rBV	2178465	1953306	83.22%	11.256%
10	9.633	1280	1283	1292	rBV	143706	128421	5.47%	0.740%
11	9.921	1329	1332	1342	rBV	549126	550769	23.47%	3.174%
12	10.710	1462	1466	1480	rBV	1232164	1246846	53.12%	7.185%
13	11.410	1581	1585	1599	rBV	734208	696382	29.67%	4.013%
14	11.933	1670	1674	1683	rBV2	82435	112240	4.78%	0.647%
15	12.721	1804	1808	1811	rBV4	27734	31169	1.33%	0.180%
16	12.992	1850	1854	1857	rBV	2701203	2347186	100.00%	13.526%
17	13.886	2002	2006	2014	rBV	139015	251485	10.71%	1.449%
18	14.051	2030	2034	2042	rVB	543670	579366	24.68%	3.339%
19	14.821	2162	2165	2170	rVB	65491	65036	2.77%	0.375%
20	14.898	2176	2178	2181	rVB	43259	36655	1.56%	0.211%
21	15.162	2220	2223	2226	rBV	57494	63583	2.71%	0.366%
22	15.527	2280	2285	2294	rVB	399988	616361	26.26%	3.552%
23	15.986	2360	2363	2368	rBV2	50821	72844	3.10%	0.420%

Sum of corrected areas: 17353310

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050219\
Data File : BF114088.D
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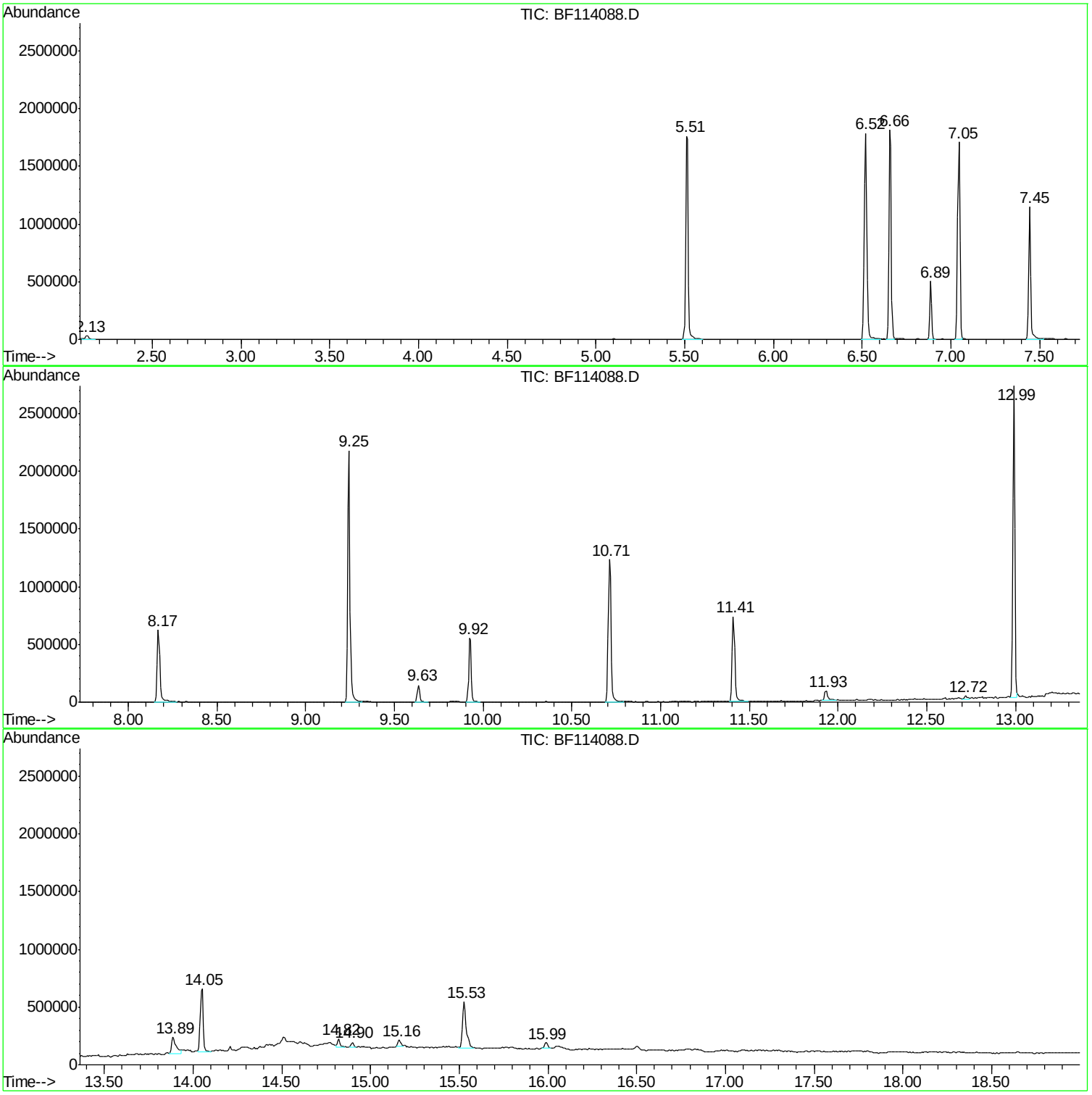
Operator : JU/SJ
Sample : K2652-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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

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Data File : BF114088.D
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Operator : JU/SJ
Sample : K2652-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

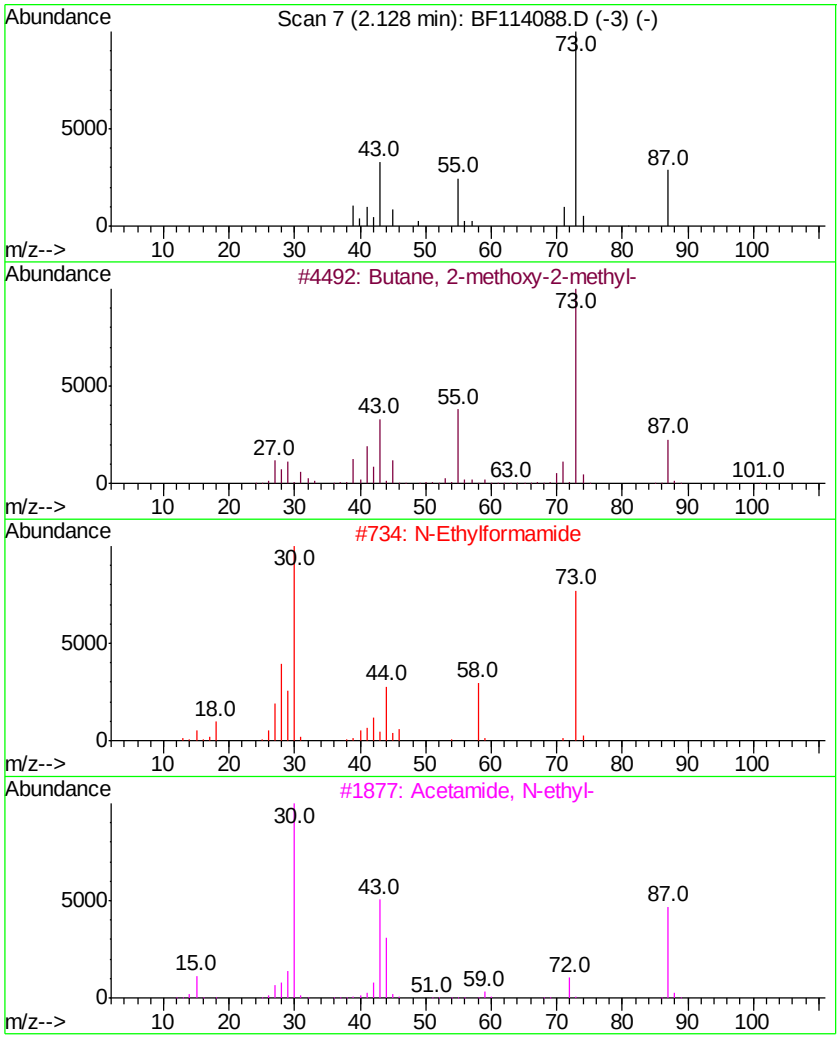
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

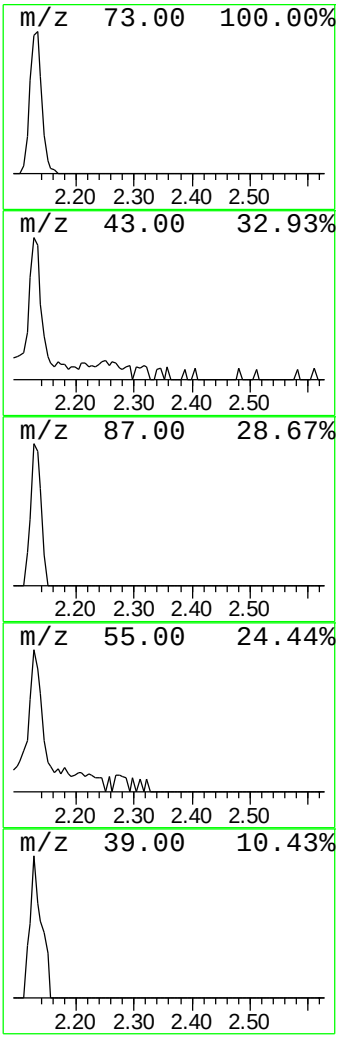
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	2.34 ng	45815	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	N-Ethylformamide	73	C3H7NO	000627-45-2	5
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5
4	1-Propene-1-thiol	74	C3H6S	000925-89-3	4
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	4





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Misc :
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Instrument : BNA_F
ClientSampleId : DRUM-1-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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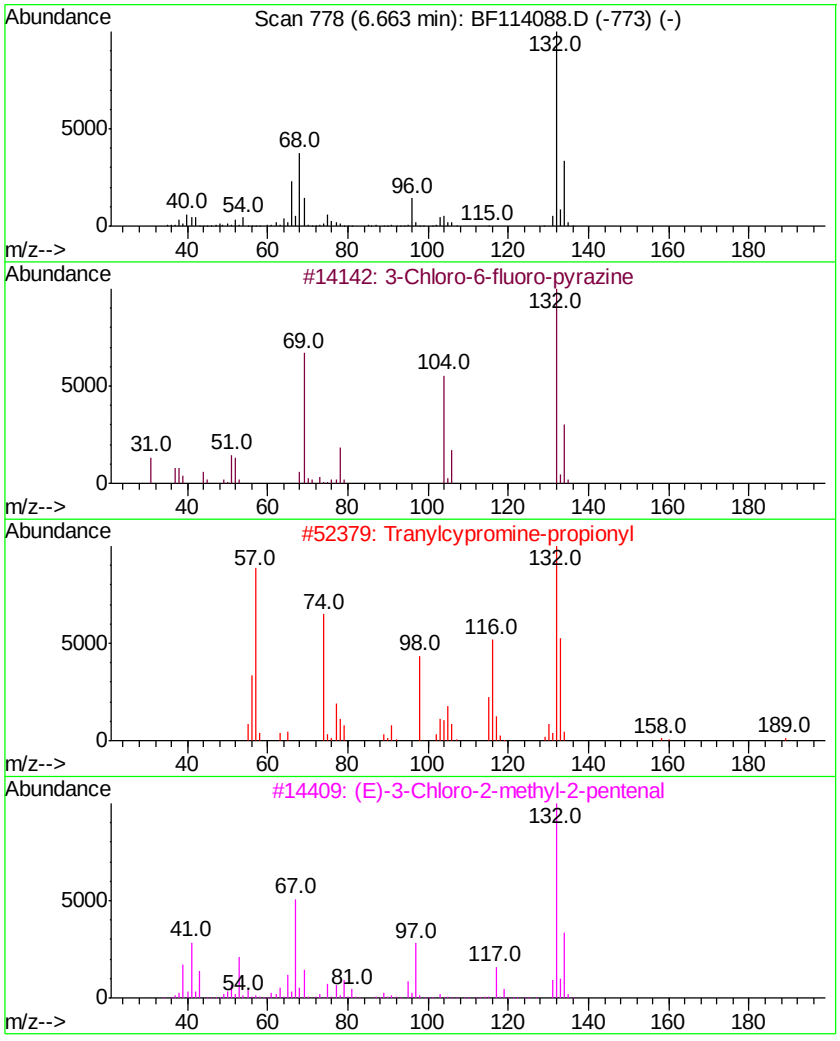
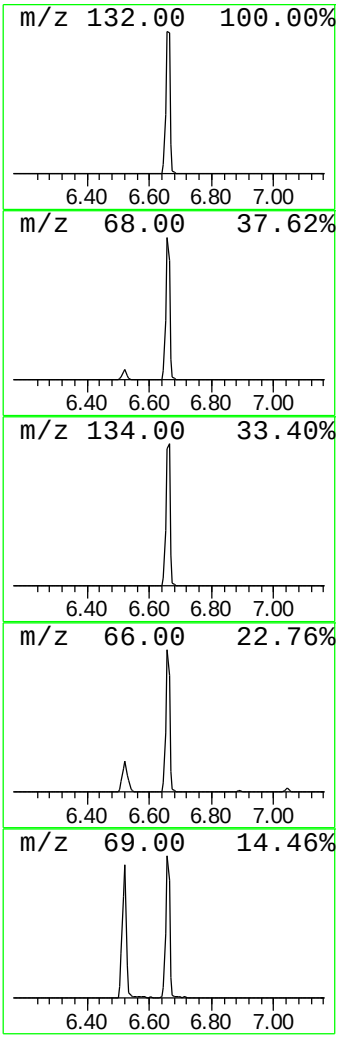
Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	85.08 ng	1668670	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

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Data File : BF114088.D
Acq On : 2 May 2019 16:58
Operator : JU/SJ
Sample : K2652-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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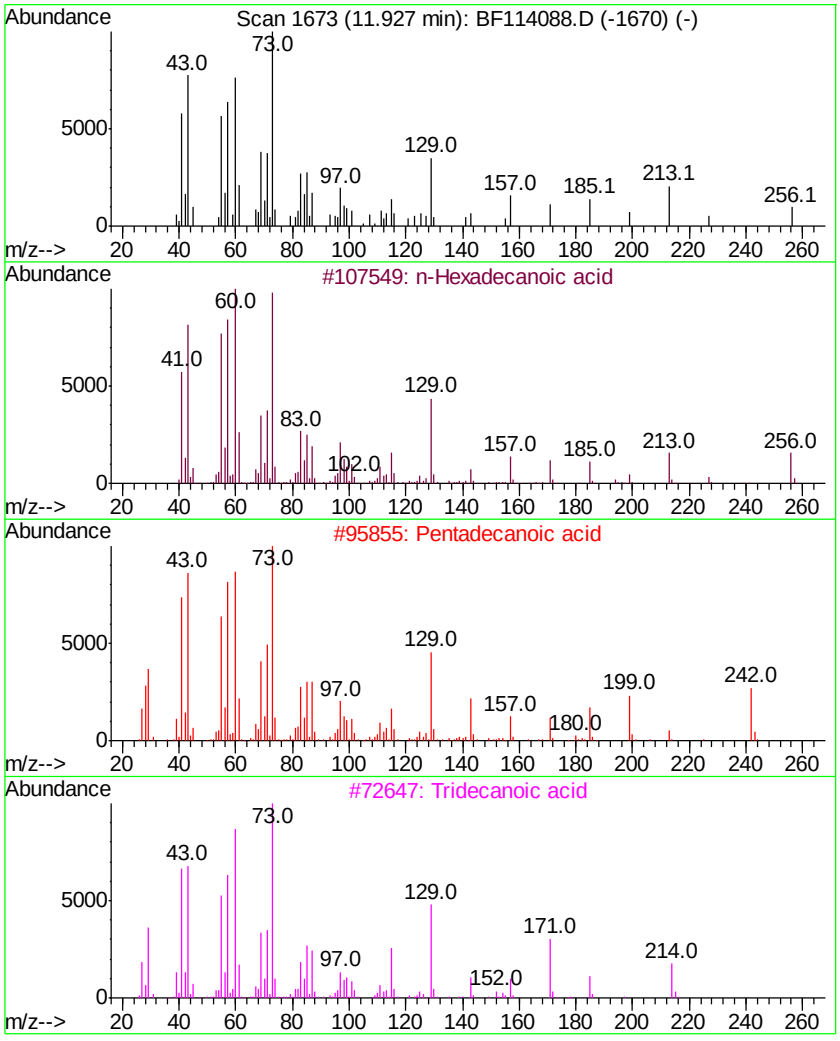
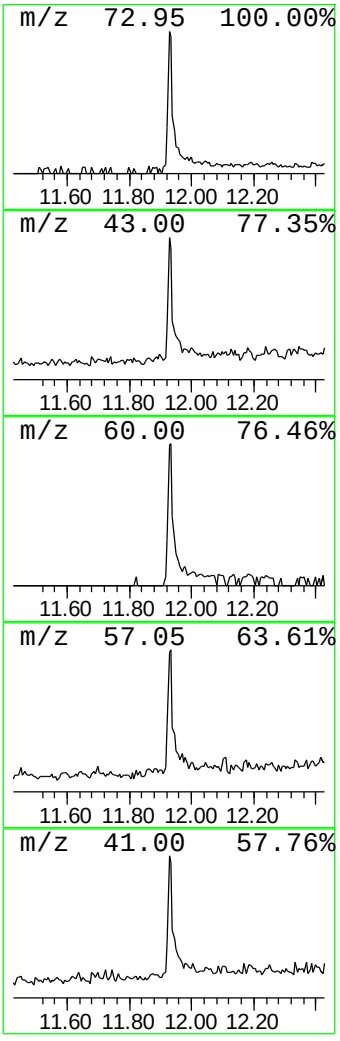
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	3.22 ng	112240	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050219\
Data File : BF114088.D
Acq On : 2 May 2019 16:58
Operator : JU/SJ
Sample : K2652-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

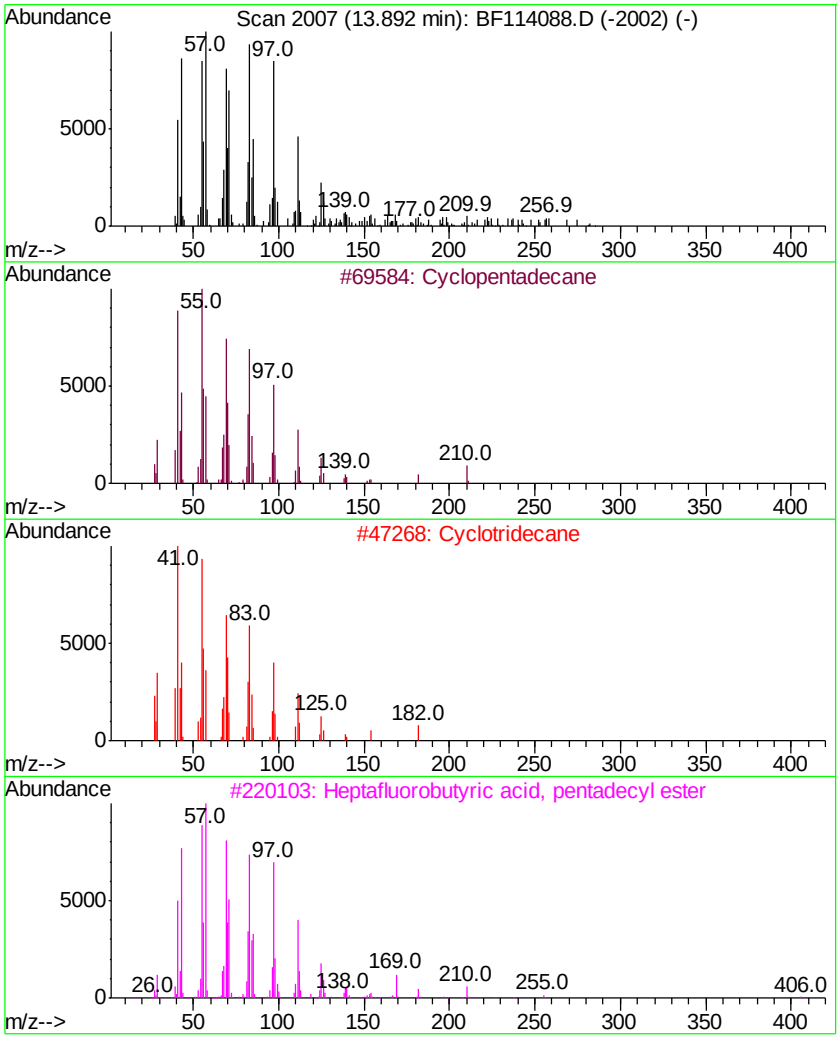
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

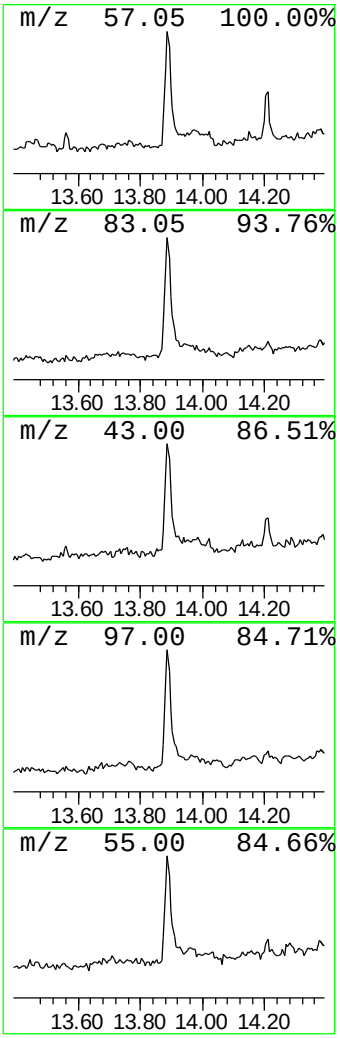
****

Peak Number 5 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	8.68 ng	251485	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	98
2	Cyclotridecane	182	C13H26	000295-02-3	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050219\
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Acq On : 2 May 2019 16:58
Operator : JU/SJ
Sample : K2652-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DRUM-1-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

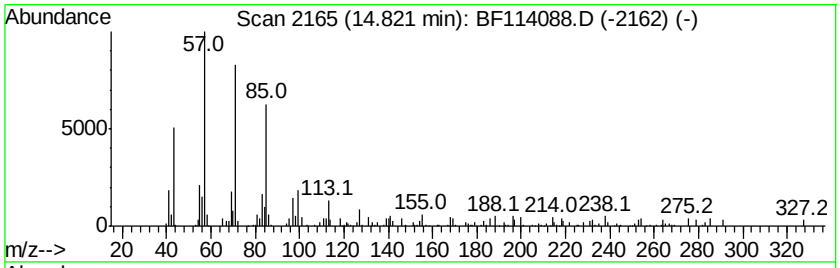
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

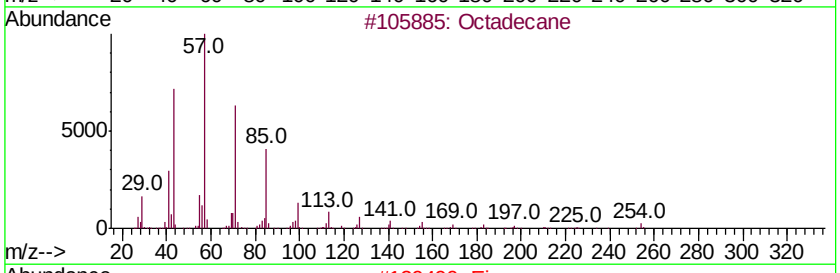
****

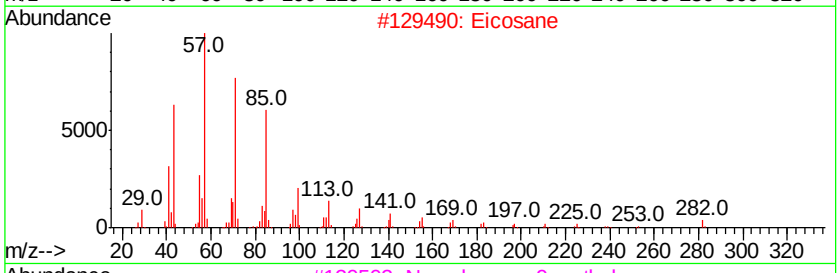
Peak Number 6 Octadecane Concentration Rank 7

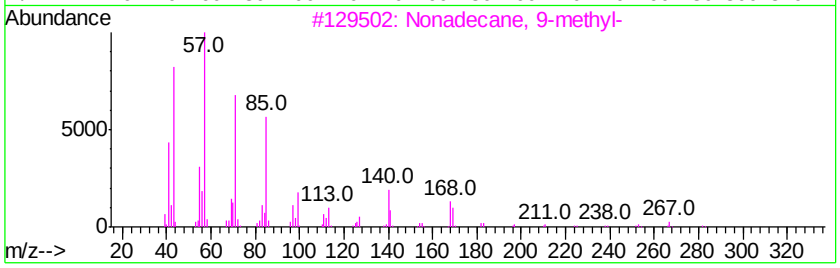
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.11 ng	65036	Perylene-d12	15.53

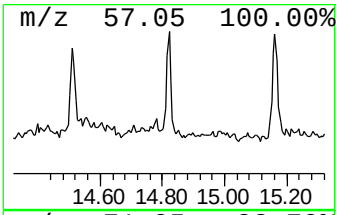
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Eicosane	282	C20H42	000112-95-8	89
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	76
4	Hexacosane	366	C26H54	000630-01-3	76
5	Octacosane	394	C28H58	000630-02-4	68

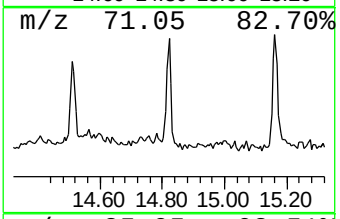


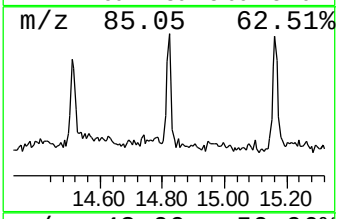


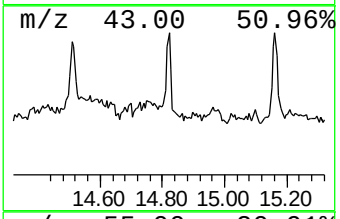


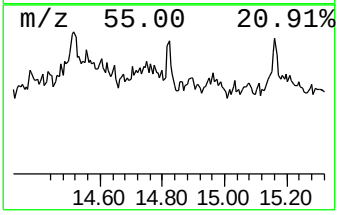












Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

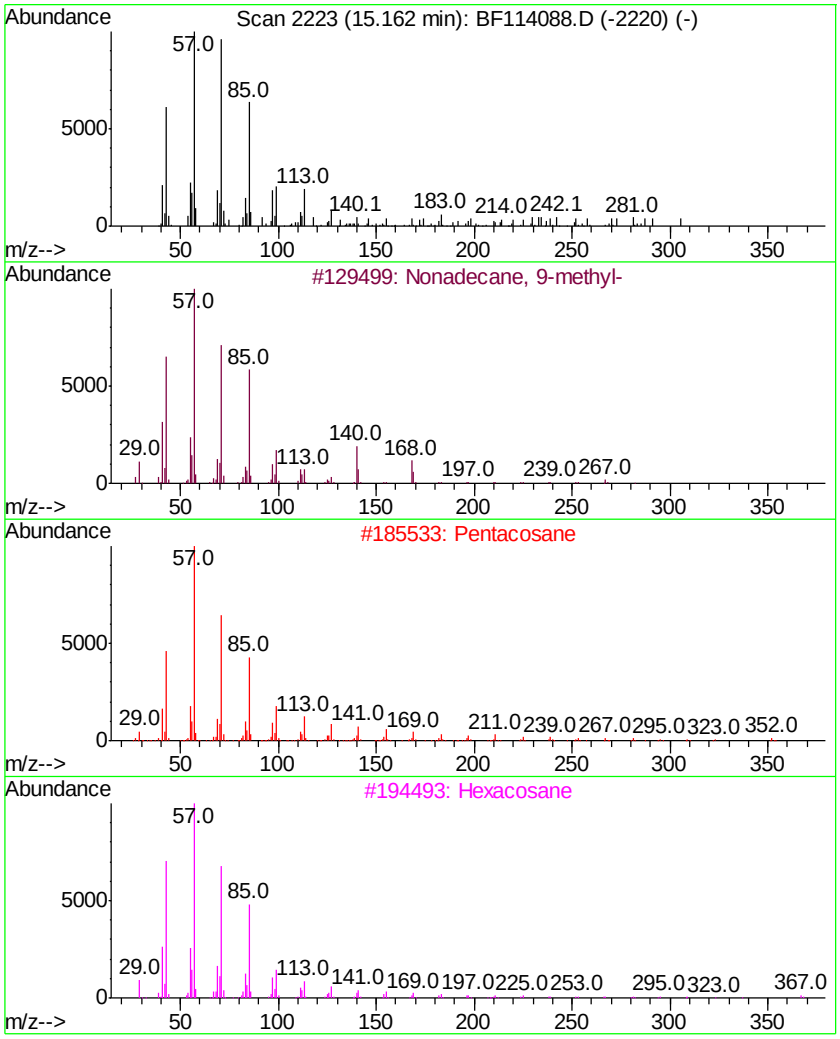
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

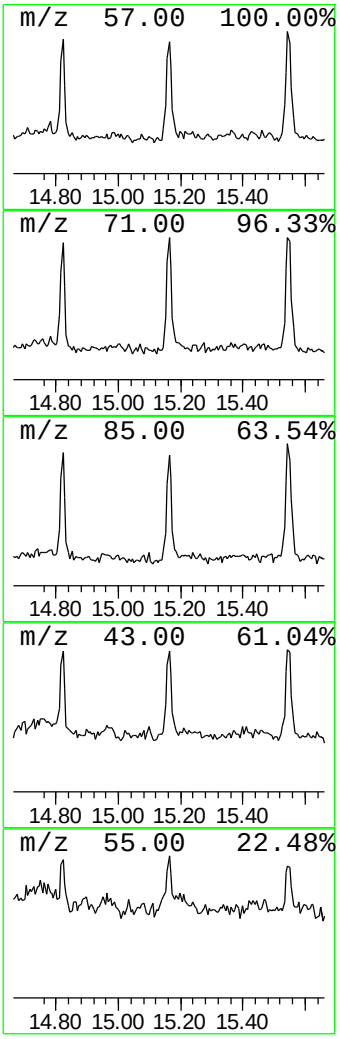
****

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.06 ng	63583	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	89
2	Pentacosane	352	C25H52	000629-99-2	80
3	Hexacosane	366	C26H54	000630-01-3	76
4	Heneicosane	296	C21H44	000629-94-7	68
5	Tetracosane	338	C24H50	000646-31-1	64





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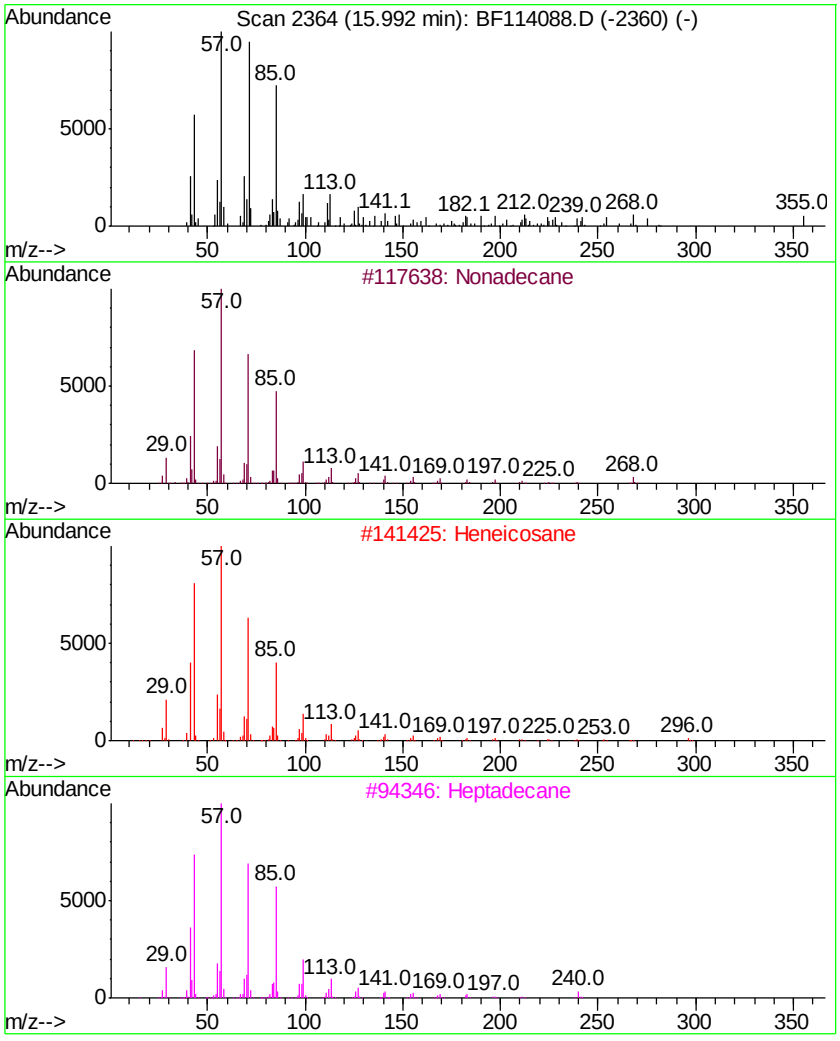
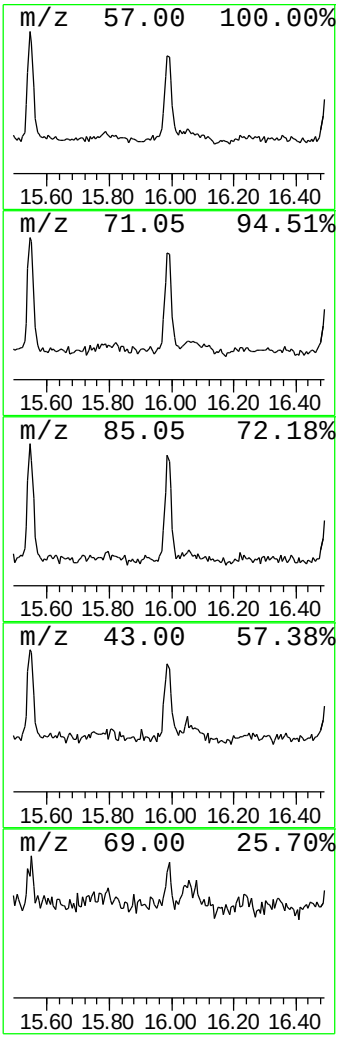
****

Peak Number 8 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.36 ng	72844	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Heneicosane	296	C21H44	000629-94-7	72
3	Heptadecane	240	C17H36	000629-78-7	72
4	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	72
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	72





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...	2.13	2.3	ng	45815	1	6.89	392250	20.0
unknown6.66	6.66	85.1	ng	1668670	1	6.89	392250	20.0
n-Hexadecanoic acid	11.93	3.2	ng	112240	4	11.41	696382	20.0
Cyclopentadecane	13.89	8.7	ng	251485	5	14.05	579366	20.0
Octadecane	14.82	2.1	ng	65036	6	15.53	616361	20.0
Nonadecane, 9-met...	15.16	2.1	ng	63583	6	15.53	616361	20.0
Nonadecane	15.99	2.4	ng	72844	6	15.53	616361	20.0