LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018933.D
Acq On : 26 Feb 2019 17:22
Operator : JU/SJ
Sample : K1620-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SB-03

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_M\METHODS\8270-BM021119.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	5.287	367	374	388	rBV	4806733	6811987	91.23%	9.068%
2	6.869	635	643	663	rBV	4323056	7396976	99.06%	9.847%
3	7.228	697	704	723	rBV	4849293	7467142	100.00%	9.941%
4	7.692	776	783	791	rBV	1365596	2142359	28.69%	2.852%
5	8.010	827	837	846	rBV	3433791	5317042	71.21%	7.078%
6	8.863	973	982	996	rBV	2500168	4229123	56.64%	5.630%
7	10.480	1249	1257	1264	rBV	1603322	2659835	35.62%	3.541%
8	11.516	1427	1433	1450	rBV	131340	323606	4.33%	0.431%
9	12.957	1670	1678	1692	rBV	4812079	6935757	92.88%	9.233%
10	13.292	1730	1735	1741	rBV4	35614	76681	1.03%	0.102%
11	13.804	1817	1822	1832	rBV	231134	362420	4.85%	0.482%
12	14.345	1904	1914	1923	rBV2	1957350	2925163	39.17%	3.894%
13	15.839	2162	2168	2185	rBV	3530402	5033127	67.40%	6.700%
14	17.098	2375	2382	2388	rBV	2056826	2925901	39.18%	3.895%
15	17.986	2528	2533	2542	rBV	493438	779653	10.44%	1.038%
16	19.268	2747	2751	2760	rBV	175360	294037	3.94%	0.391%
17	19.727	2824	2829	2841	rBV	5770800	7069844	94.68%	9.412%
18	20.527	2962	2965	2969	rBV	80090	94391	1.26%	0.126%
19	20.992	3040	3044	3054	rBV	488110	721381	9.66%	0.960%
20	21.197	3075	3079	3083	rBV	635272	710366	9.51%	0.946%
21	21.292	3090	3095	3105	rBV	2764728	3585136	48.01%	4.773%
22	21.427	3115	3118	3122	rBV	221605	240805	3.22%	0.321%
23	21.856	3188	3191	3196	rBV	288805	381452	5.11%	0.508%
24	22.321	3267	3270	3277	rVB	482238	600436	8.04%	0.799%
25	22.827	3352	3356	3361	rBV	484464	656672	8.79%	0.874%
26	23.391	3449	3452	3460	rVB	441204	704397	9.43%	0.938%
27	23.544	3471	3478	3487	rVB	1981780	3838610	51.41%	5.110%
28	24.038	3558	3562	3569	rVB	441236	833756	11.17%	1.110%

Sum of corrected areas: 75118055

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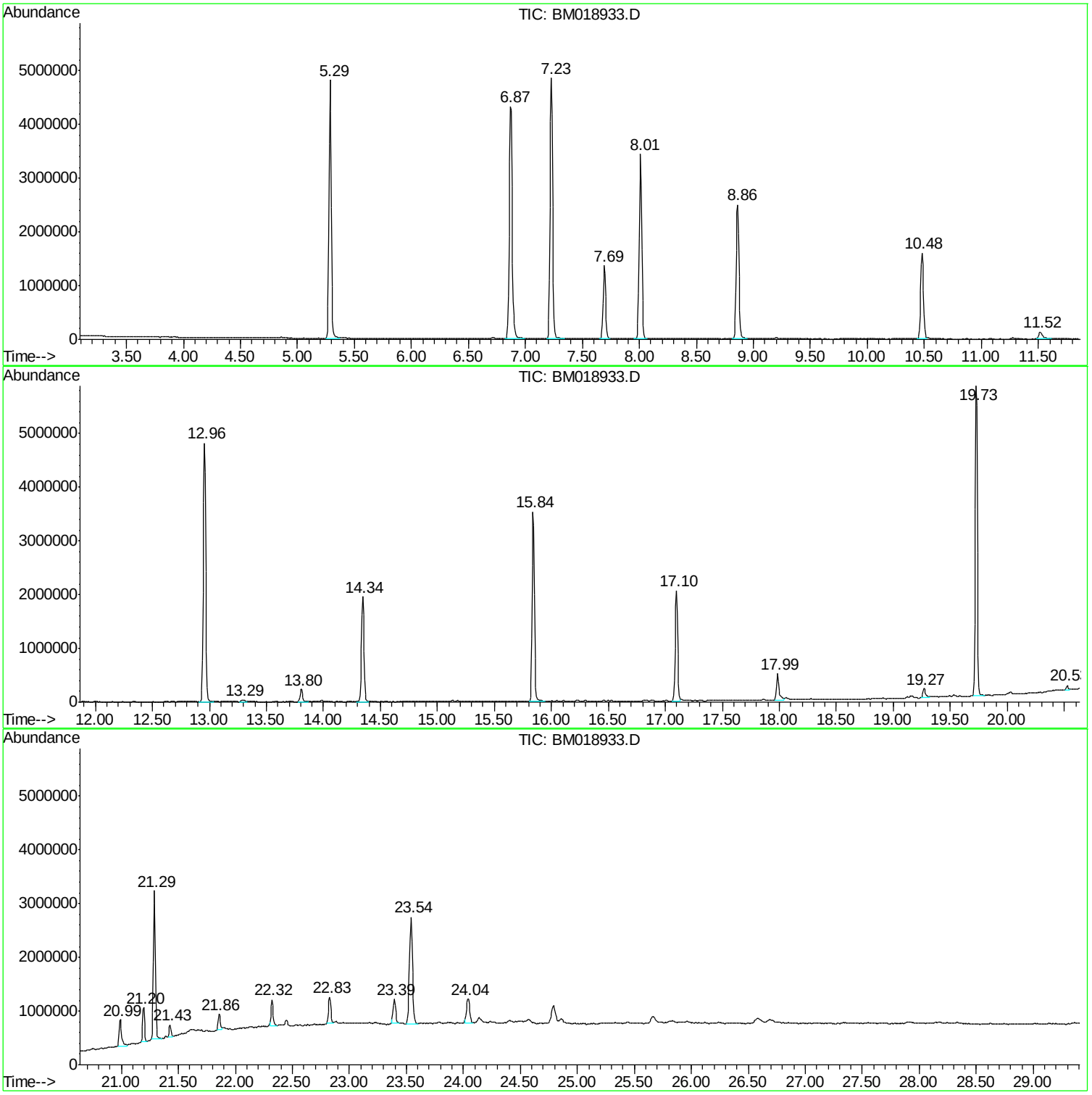
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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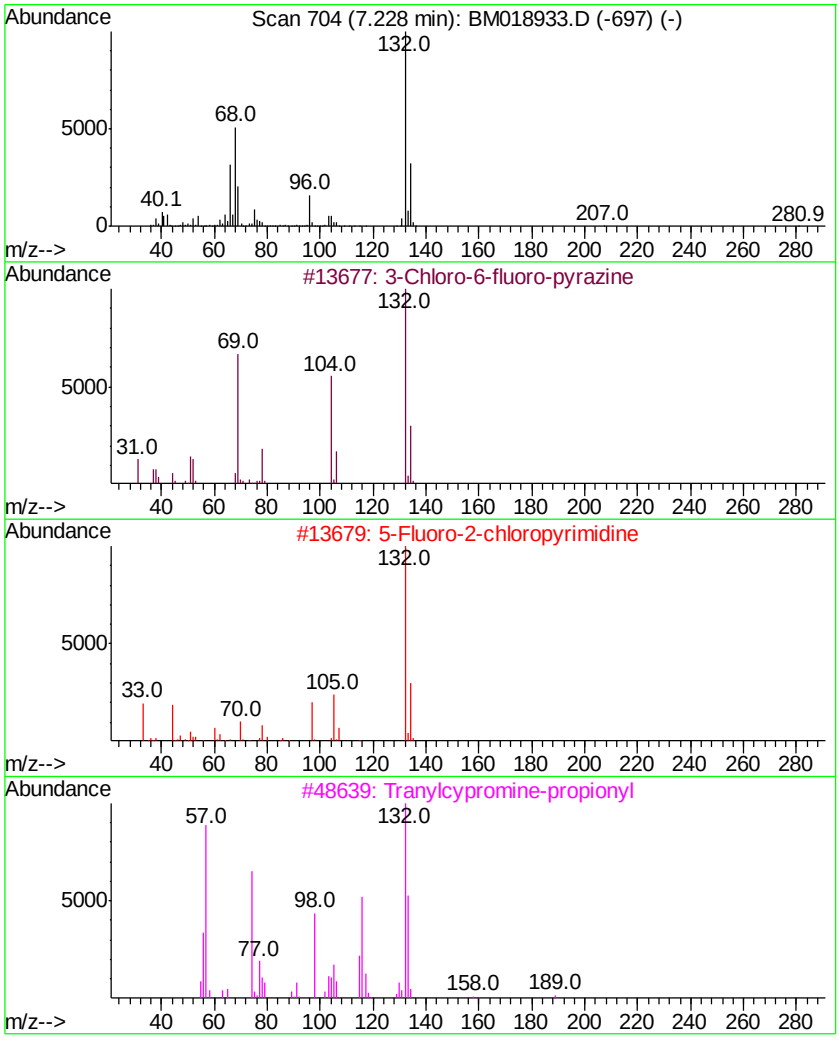
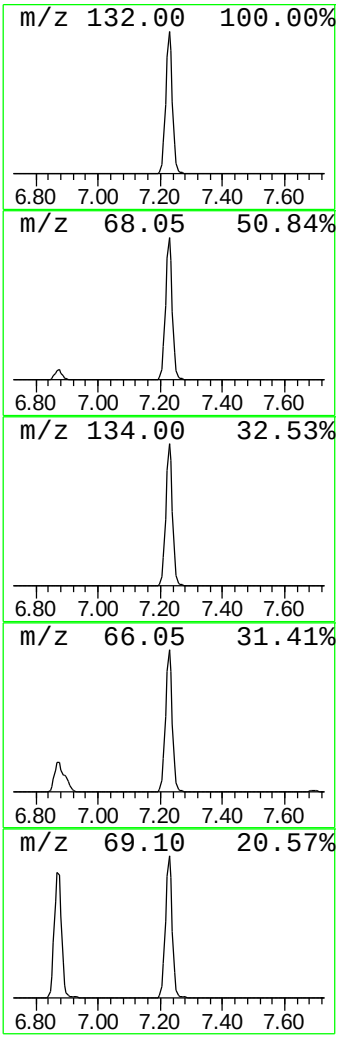
Peak Number 1 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	69.71 ng	7467140	1,4-Dichlorobenzene-d4	7.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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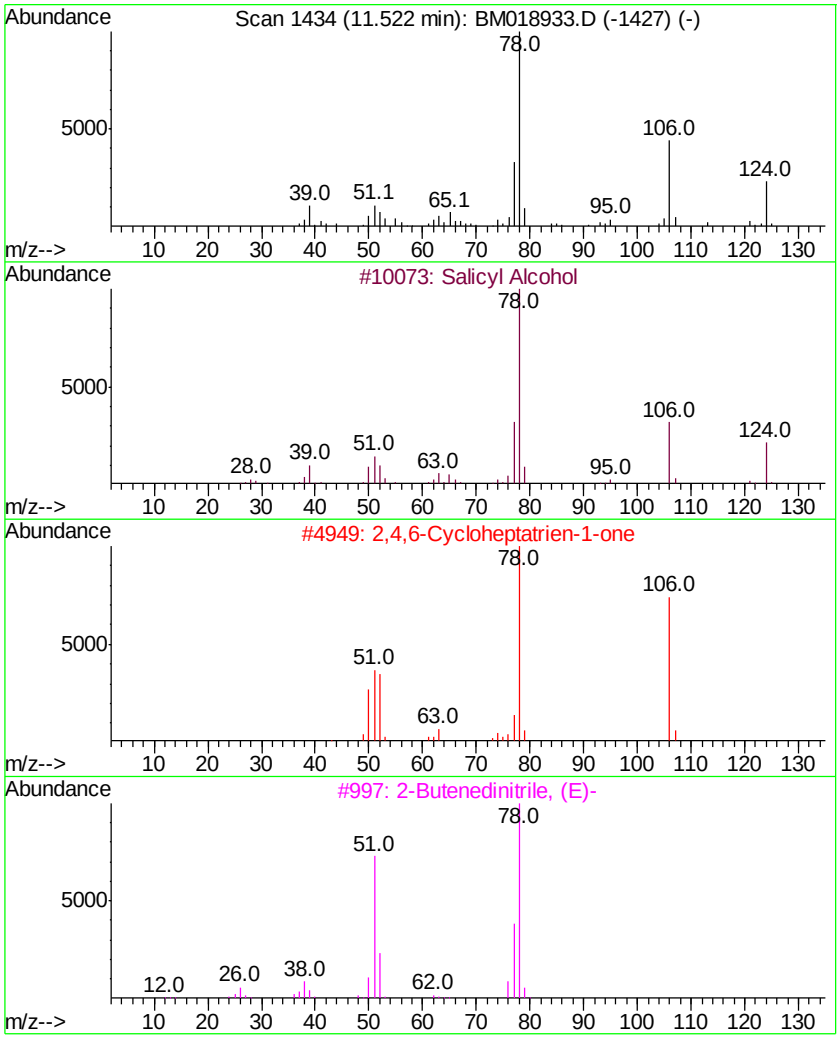
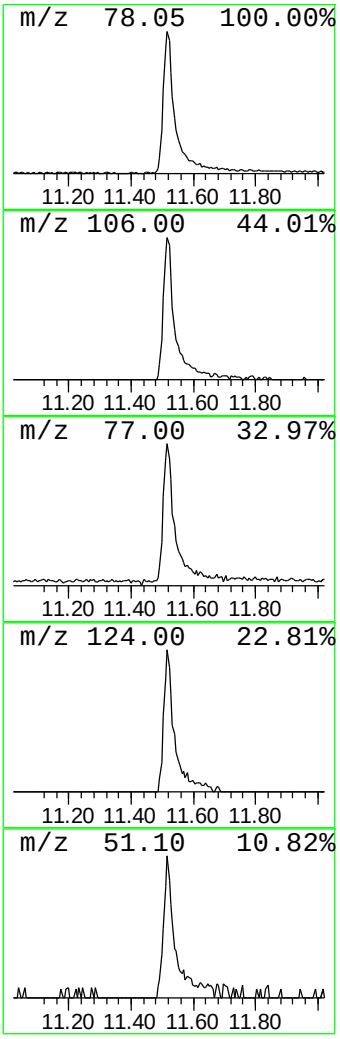
Peak Number 3 Salicyl Alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	2.43 ng	323606	Naphthalene-d8	10.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Salicyl Alcohol	124	C7H8O2	000090-01-7	91
2	2,4,6-Cycloheptatrien-1-one	106	C7H6O	000539-80-0	87
3	2-Butenedinitrile, (E)-	78	C4H2N2	000764-42-1	64
4	1,3-Hexadien-5-yne	78	C6H6	010420-90-3	50
5	Benzene	78	C6H6	000071-43-2	50





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Instrument : BNA_M
ClientSampleId : SB-03

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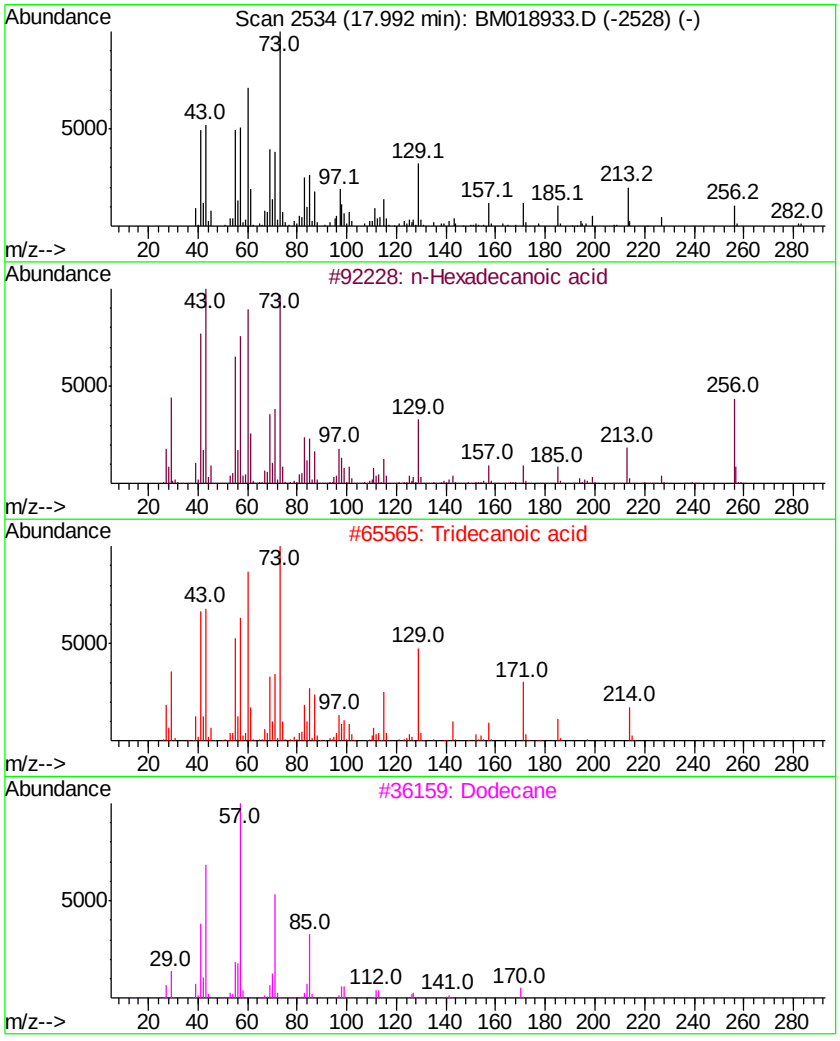
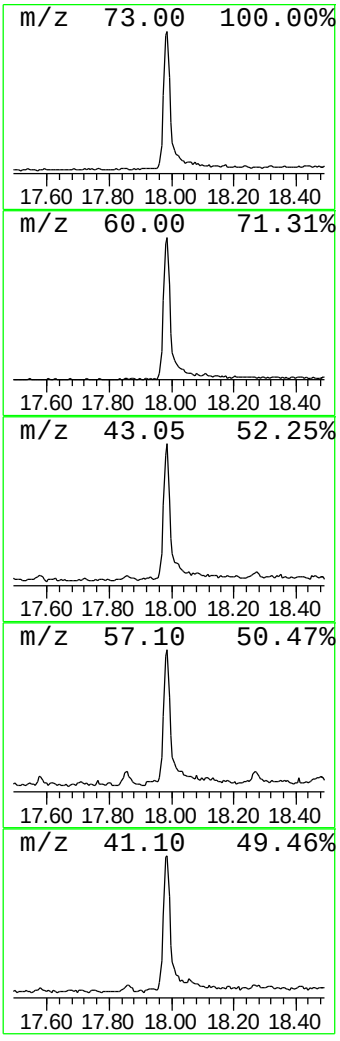
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	5.33 ng	779653	Phenanthrene-d10	17.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	60
3	Dodecane	170	C12H26	000112-40-3	18
4	Eicosane	282	C20H42	000112-95-8	18
5	Tetradecane	198	C14H30	000629-59-4	18





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Instrument : BNA_M
ClientSampleId : SB-03

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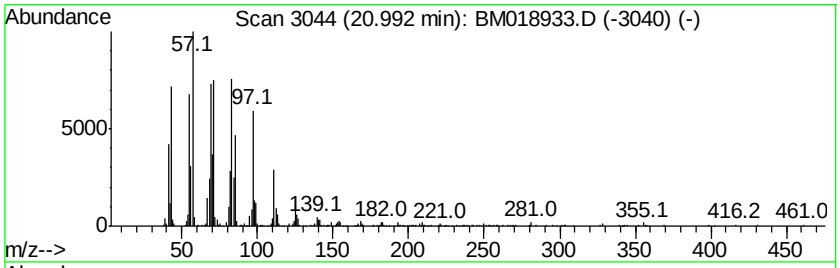
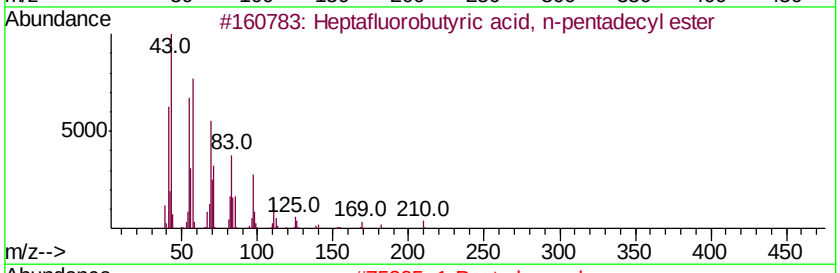
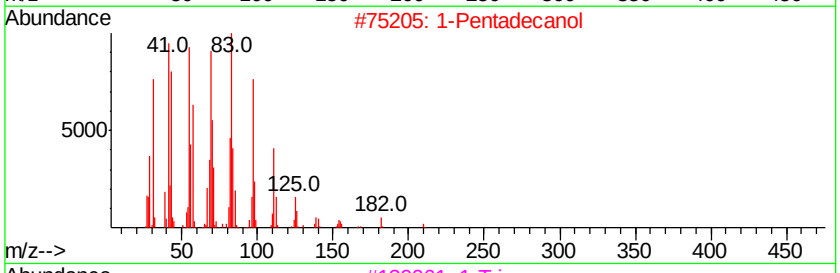
Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 5

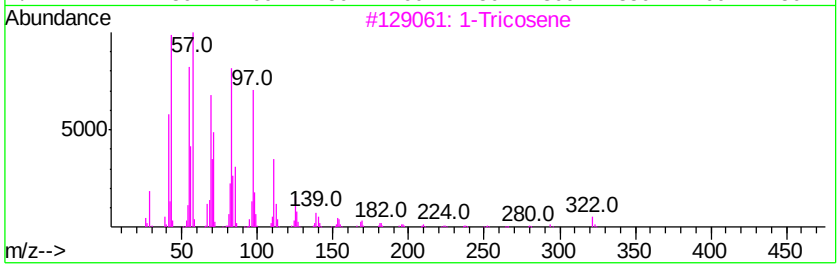
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.99	4.02 ng	721381	Chrysene-d12	21.29

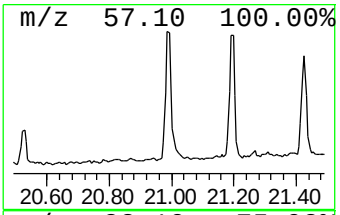
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	76
2	1-Pentadecanol	228	C15H32O	000629-76-5	64
3	1-Tricosene	322	C23H46	018835-32-0	62
4	1-Octadecanol	270	C18H38O	000112-92-5	62
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	62

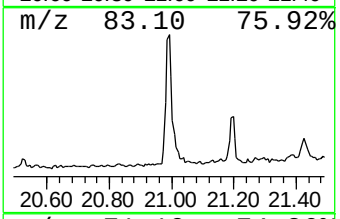


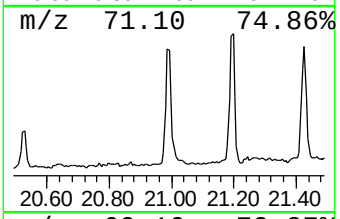


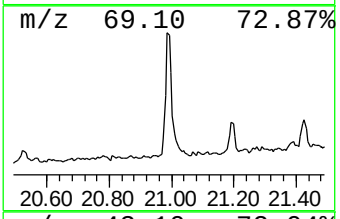


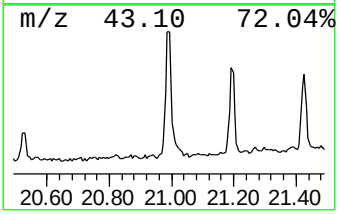












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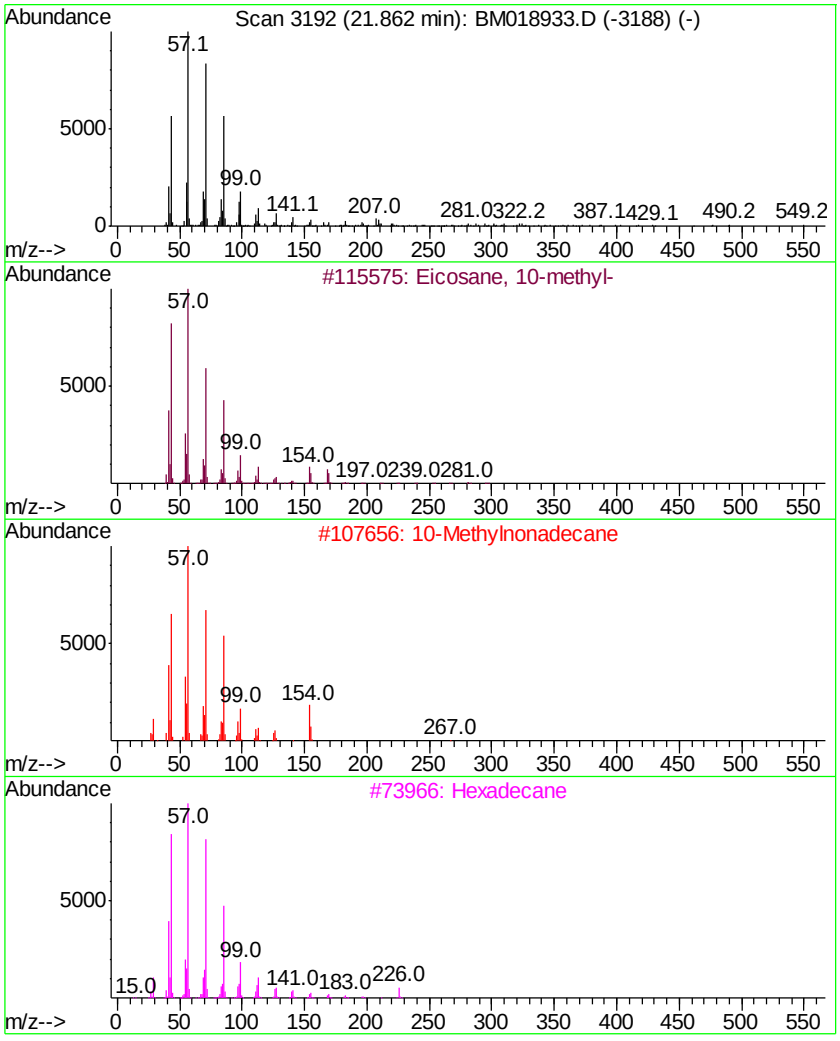
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

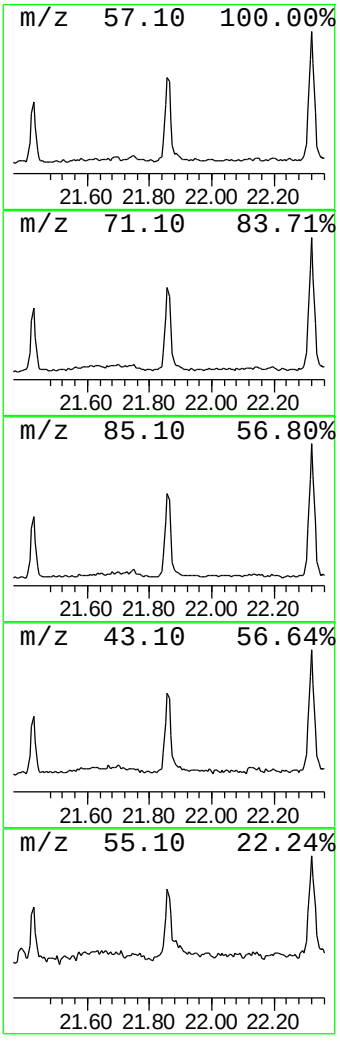
****

Peak Number 6 Eicosane, 10-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	2.13 ng	381452	Chrysene-d12	21.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
2	10-Methylnonadecane	282	C20H42	056862-62-5	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	Heptacosane	380	C27H56	000593-49-7	87





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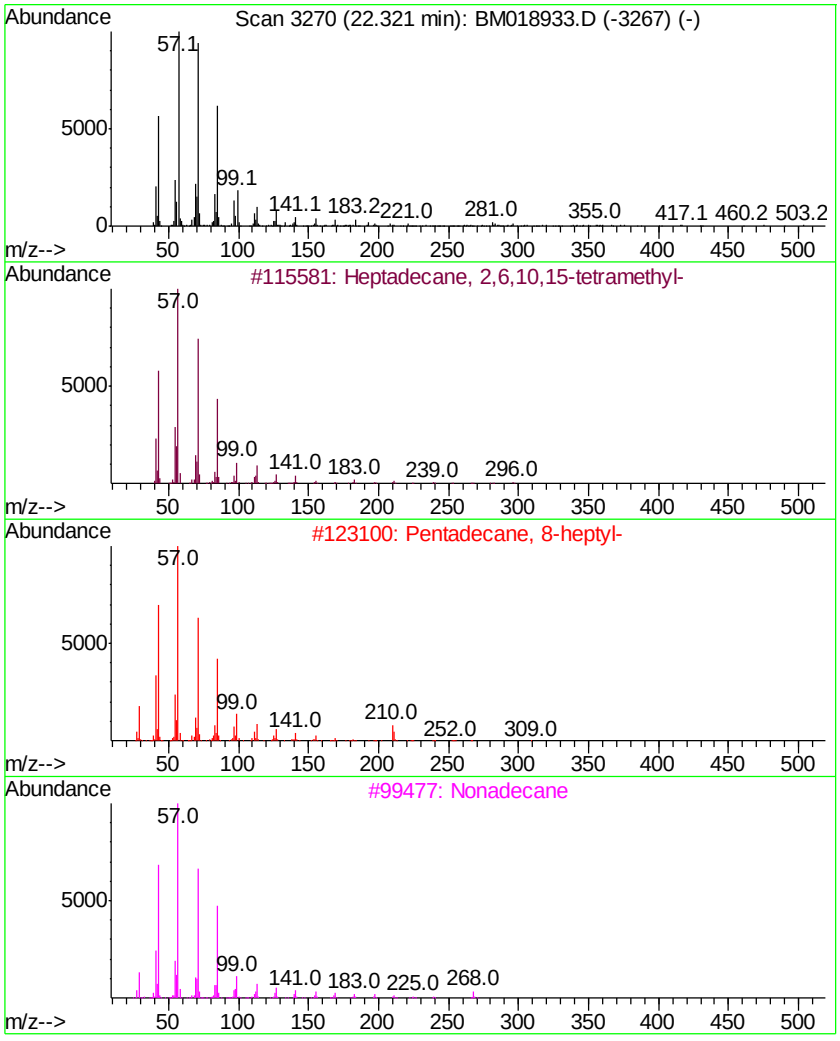
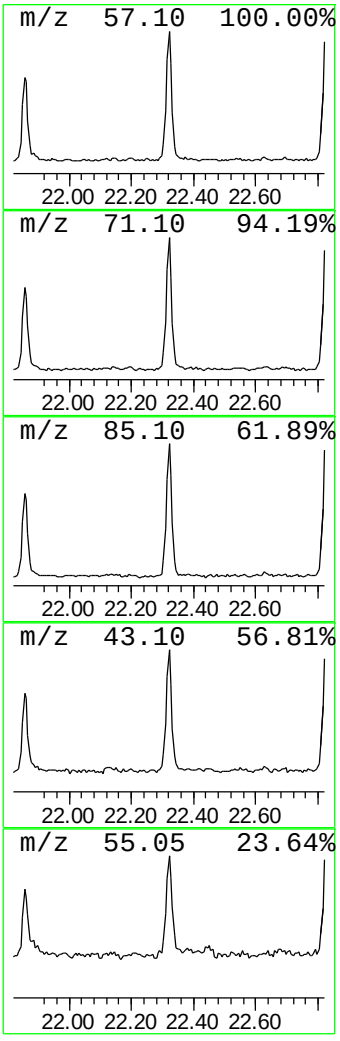
****

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.32	3.35 ng	600436	Chrysene-d12	21.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Nonadecane	268	C19H40	000629-92-5	86
4	Tetradecane	198	C14H30	000629-59-4	80
5	Octadecane	254	C18H38	000593-45-3	80





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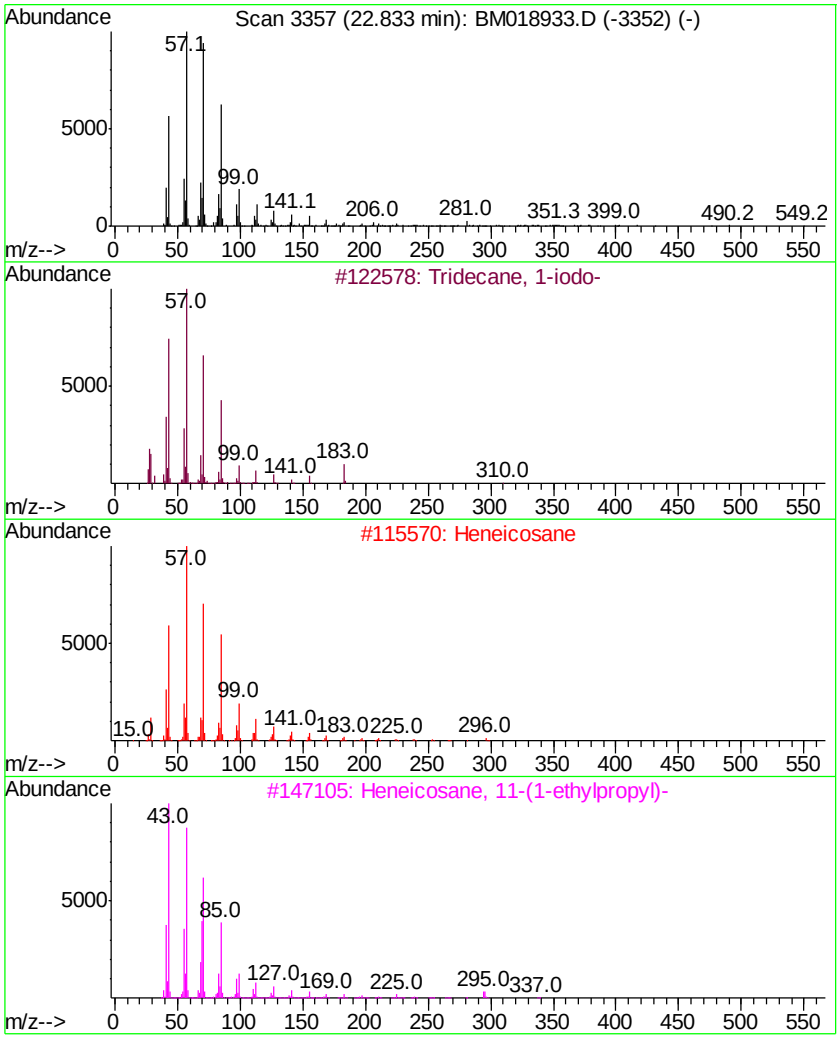
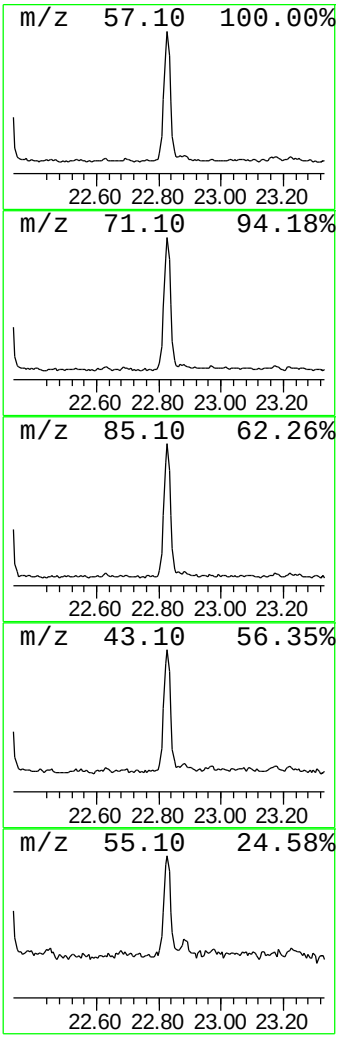
****

Peak Number 8 Tridecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.83	3.42 ng	656672	Perylene-d12	23.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Docosane, 5-butyl-	366	C26H54	055282-16-1	86





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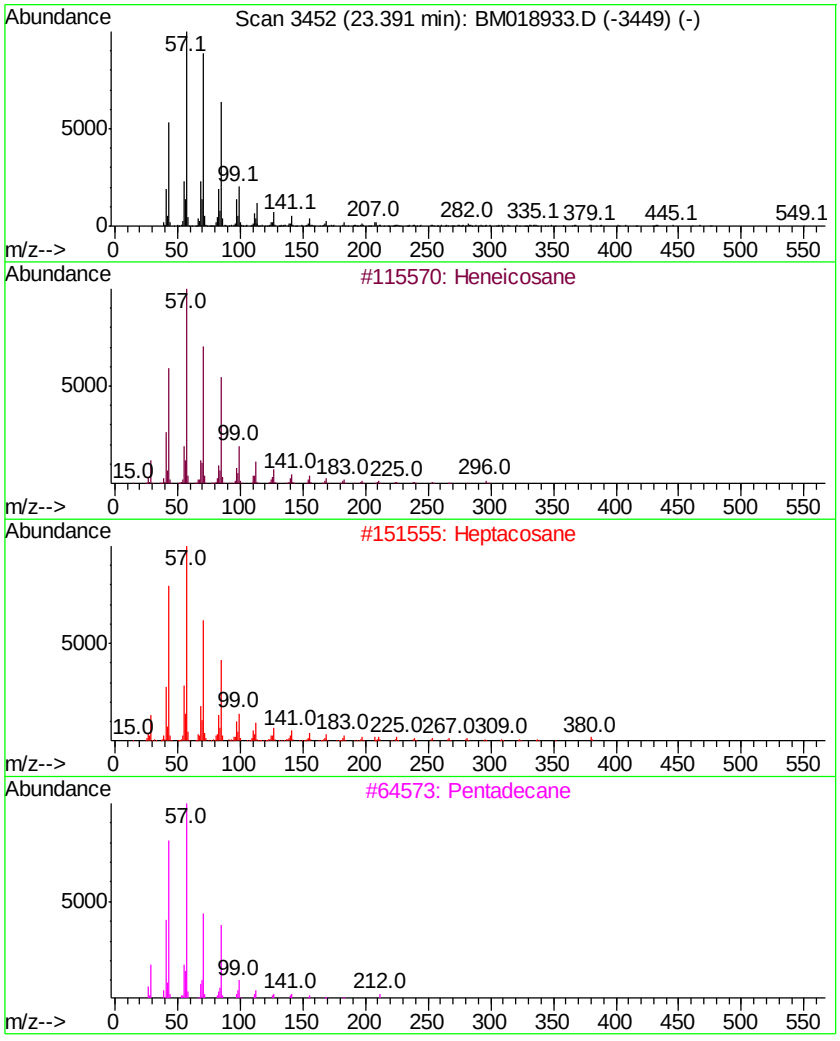
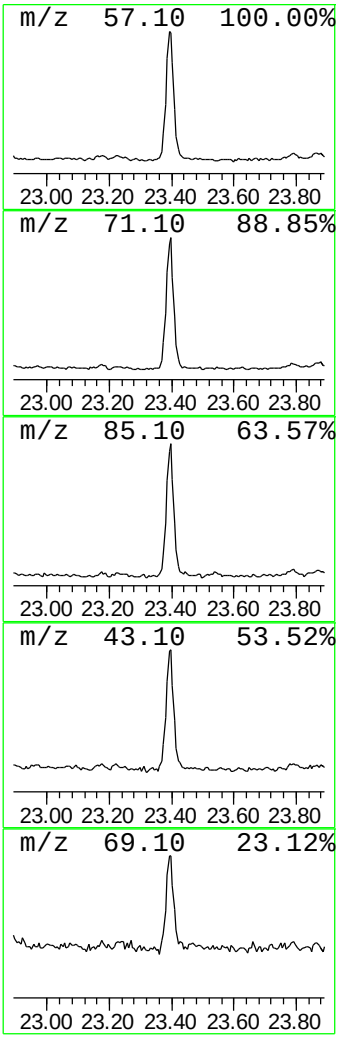
Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.39	3.67 ng	704397	Perylene-d12	23.54

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	Pentadecane	212	C15H32	000629-62-9	87
4	Octacosane	394	C28H58	000630-02-4	86
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





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Sample : K1620-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

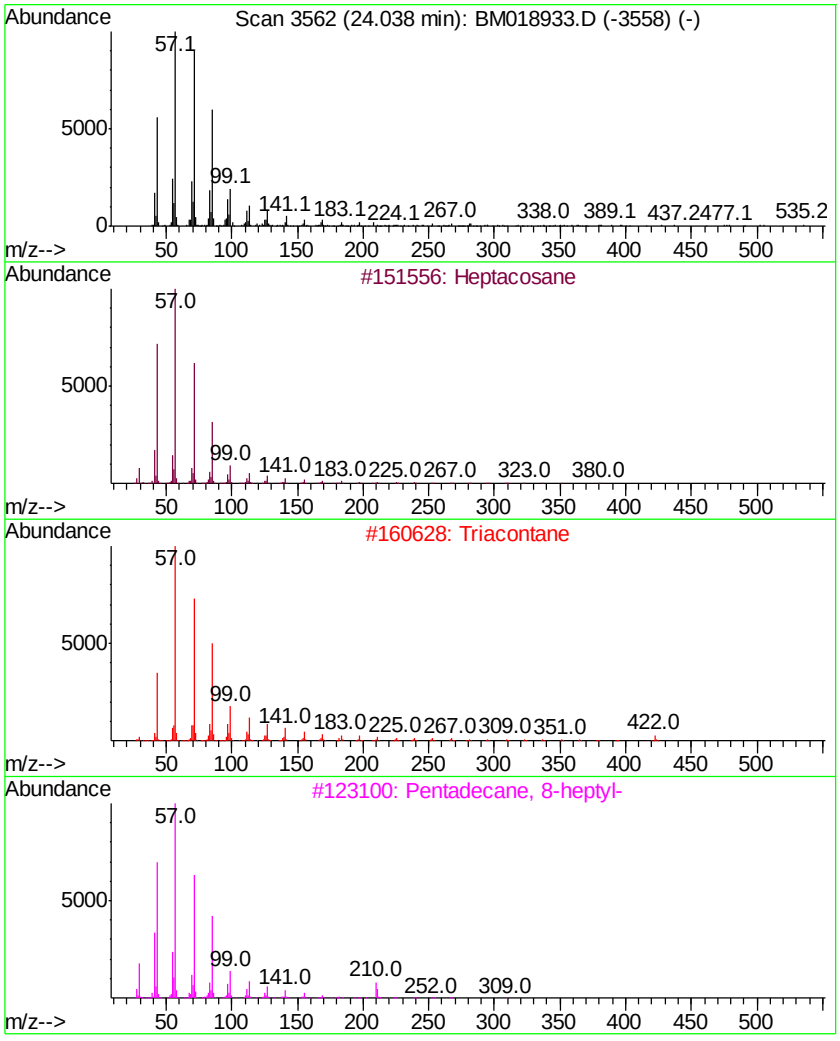
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

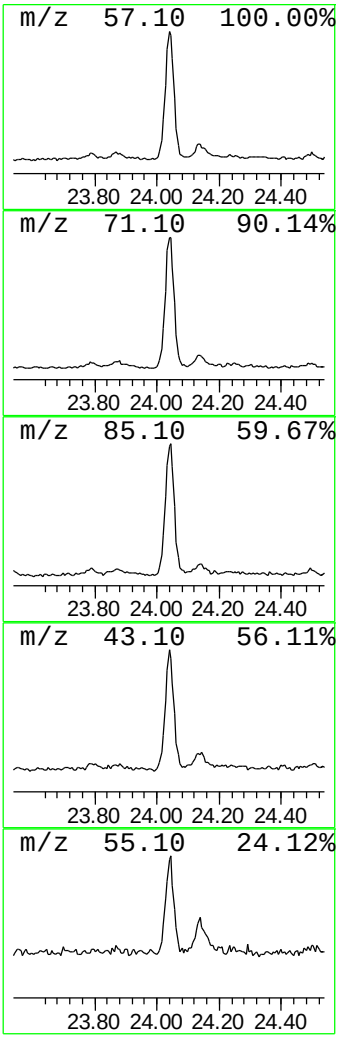
****

Peak Number 10 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.04	4.34 ng	833756	Perylene-d12	23.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	93
2	Triacontane	422	C30H62	000638-68-6	91
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Nonacosane	408	C29H60	000630-03-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM022619\
Data File : BM018933.D
Acq On : 26 Feb 2019 17:22
Operator : JU/SJ
Sample : K1620-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.23	7.23	69.7	ng	7467140	1	7.69	2142360	20.0
Salicyl Alcohol	11.52	2.4	ng	323606	2	10.48	2659840	20.0
n-Hexadecanoic acid	17.99	5.3	ng	779653	4	17.10	2925900	20.0
Heptafluorobutyri...	20.99	4.0	ng	721381	5	21.29	3585140	20.0
Eicosane, 10-methyl-	21.86	2.1	ng	381452	5	21.29	3585140	20.0
Heptadecane, 2,6,...	22.32	3.4	ng	600436	5	21.29	3585140	20.0
Tridecane, 1-iodo-	22.83	3.4	ng	656672	6	23.54	3838610	20.0
Heneicosane	23.39	3.7	ng	704397	6	23.54	3838610	20.0
Heptacosane	24.04	4.3	ng	833756	6	23.54	3838610	20.0