LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053119\
Data File : BM020641.D
Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-8

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-BM053119.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	3.069	9	14	28	rVB	2456820	2843019	21.63%	2.693%
2	5.416	406	413	427	rBV	6688696	9837583	74.86%	9.318%
3	6.998	673	682	698	rBV	6644966	11127766	84.67%	10.540%
4	7.369	737	745	753	rBV	7007943	11123138	84.64%	10.536%
5	7.834	817	824	831	rBV	1279611	1993693	15.17%	1.888%
6	8.151	871	878	886	rBV	4934324	8113635	61.74%	7.685%
7	8.998	1012	1022	1033	rBV	4029748	6773482	51.54%	6.416%
8	10.628	1291	1299	1306	rBV	1569188	2700613	20.55%	2.558%
9	11.645	1466	1472	1481	rBV	198238	349905	2.66%	0.331%
10	13.092	1711	1718	1725	rBV	8966269	13141777	100.00%	12.448%
11	13.927	1852	1860	1869	rBV	901222	1236133	9.41%	1.171%
12	14.469	1945	1952	1964	rVB2	1960800	3036826	23.11%	2.876%
13	15.957	2198	2205	2226	rBV	5398641	7907125	60.17%	7.490%
14	17.215	2412	2419	2426	rBV2	2019253	2892114	22.01%	2.739%
15	18.110	2566	2571	2581	rBV	546399	797302	6.07%	0.755%
16	19.386	2784	2788	2799	rBV	182317	311249	2.37%	0.295%
17	19.839	2859	2865	2870	rBV	9828553	11758769	89.48%	11.138%
18	21.103	3076	3080	3091	rBV	1065697	1452847	11.06%	1.376%
19	21.386	3123	3128	3134	rBV	2188467	2866765	21.81%	2.715%
20	21.551	3153	3156	3161	rVB	171202	182958	1.39%	0.173%
21	21.998	3228	3232	3236	rBV2	181209	260209	1.98%	0.246%
22	22.474	3309	3313	3317	rBV	184092	240268	1.83%	0.228%
23	22.603	3331	3335	3341	rVB	468297	647756	4.93%	0.614%
24	22.997	3398	3402	3407	rBV	186143	267999	2.04%	0.254%
25	23.592	3499	3503	3509	rVB	165836	264290	2.01%	0.250%
26	23.680	3511	3518	3526	rVB	1662984	3097726	23.57%	2.934%
27	24.350	3628	3632	3641	rVB2	190565	349457	2.66%	0.331%

Sum of corrected areas: 105574404

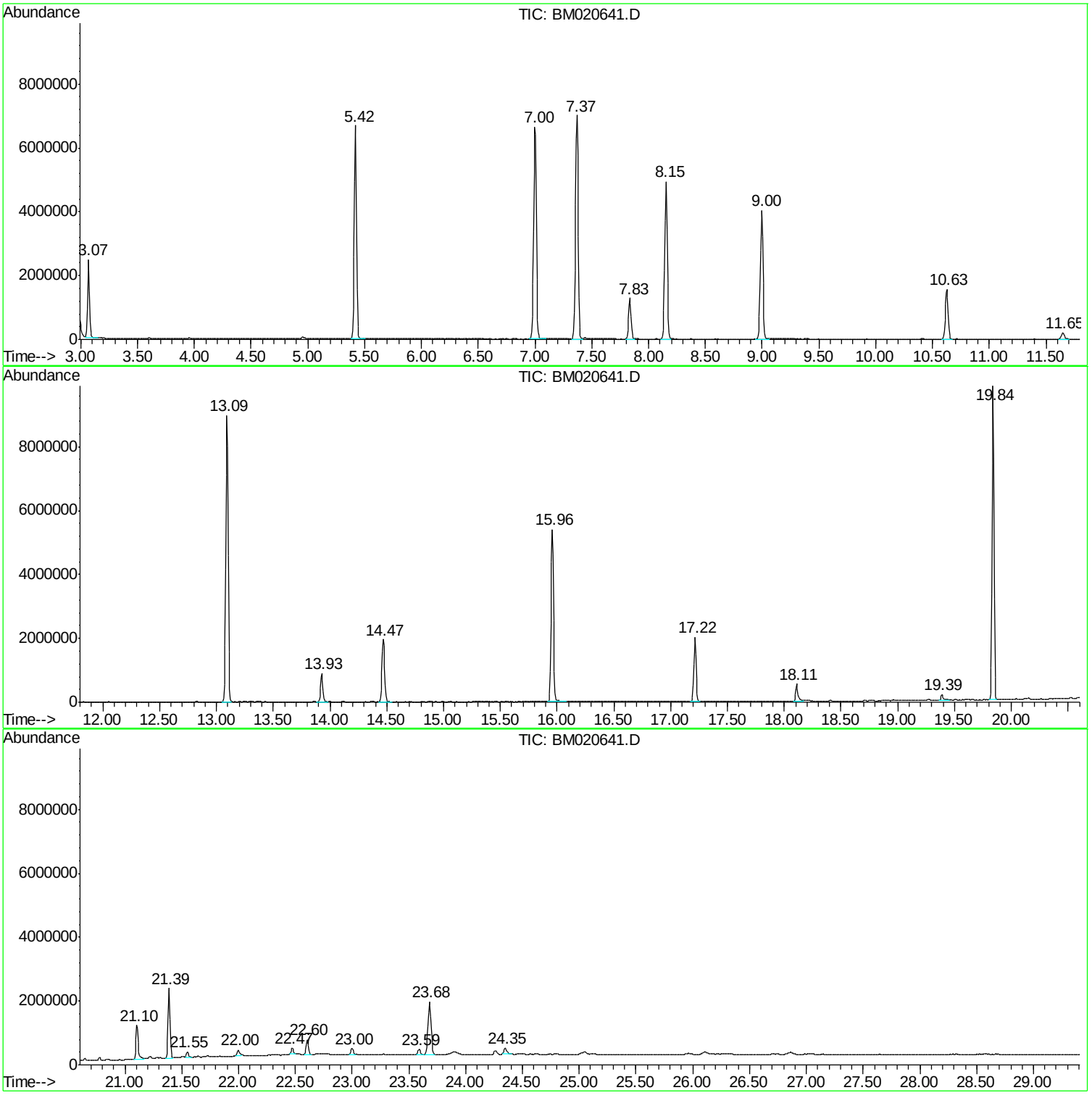
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053119\
Data File : BM020641.D
Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053119\
Data File : BM020641.D
Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

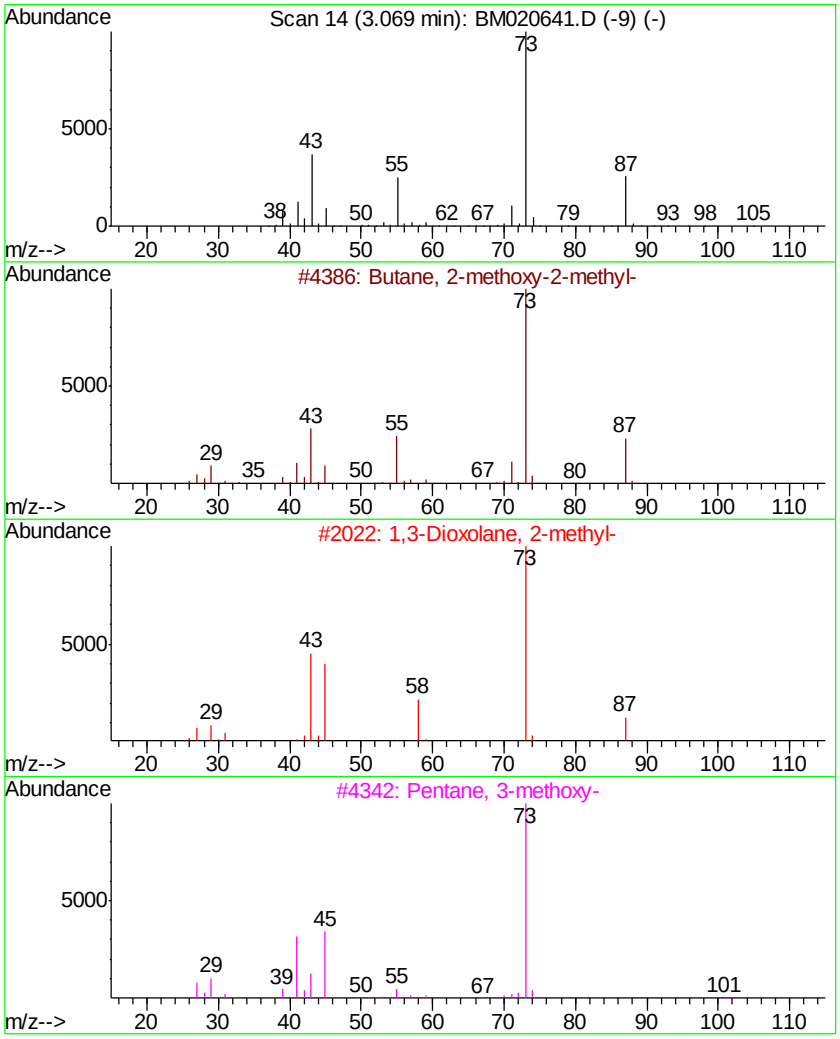
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

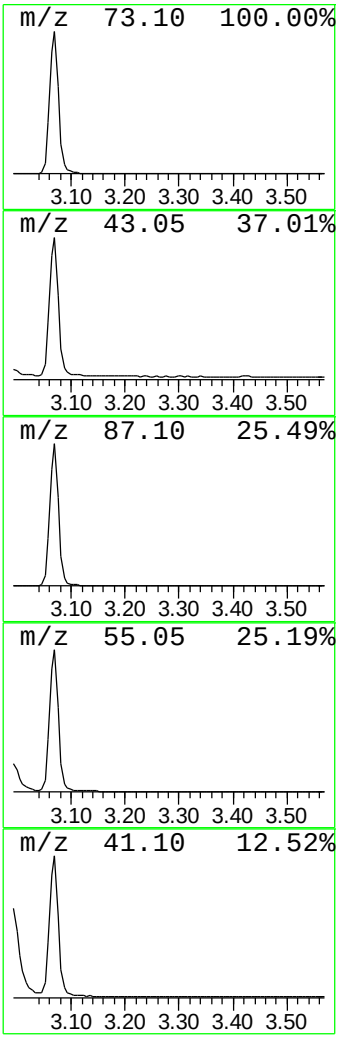
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.07	28.52 ng	2843020	1,4-Dichlorobenzene-d4	7.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Library Search Compound Report

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Data File : BM020641.D
Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

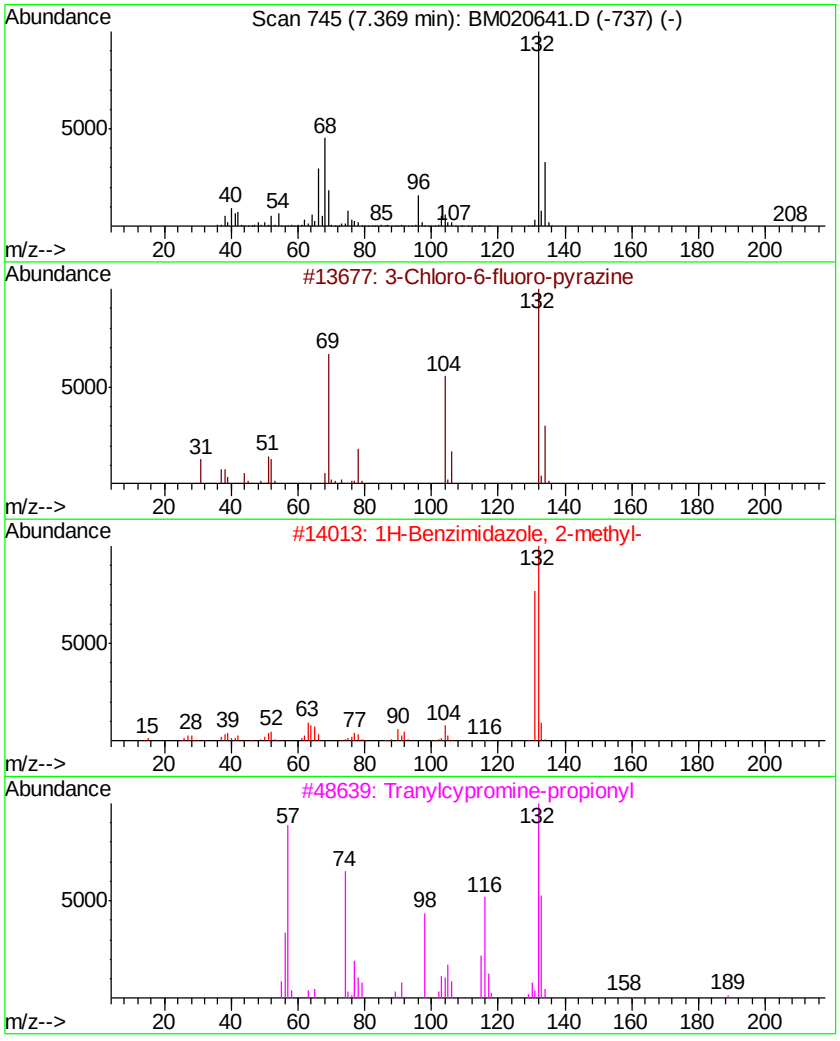
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

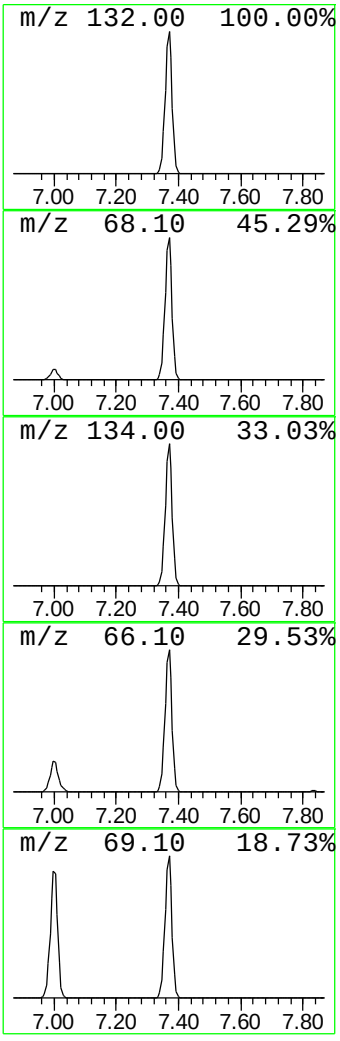
****

Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	111.58 ng	11123100	1,4-Dichlorobenzene-d4	7.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053119\
Data File : BM020641.D
Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

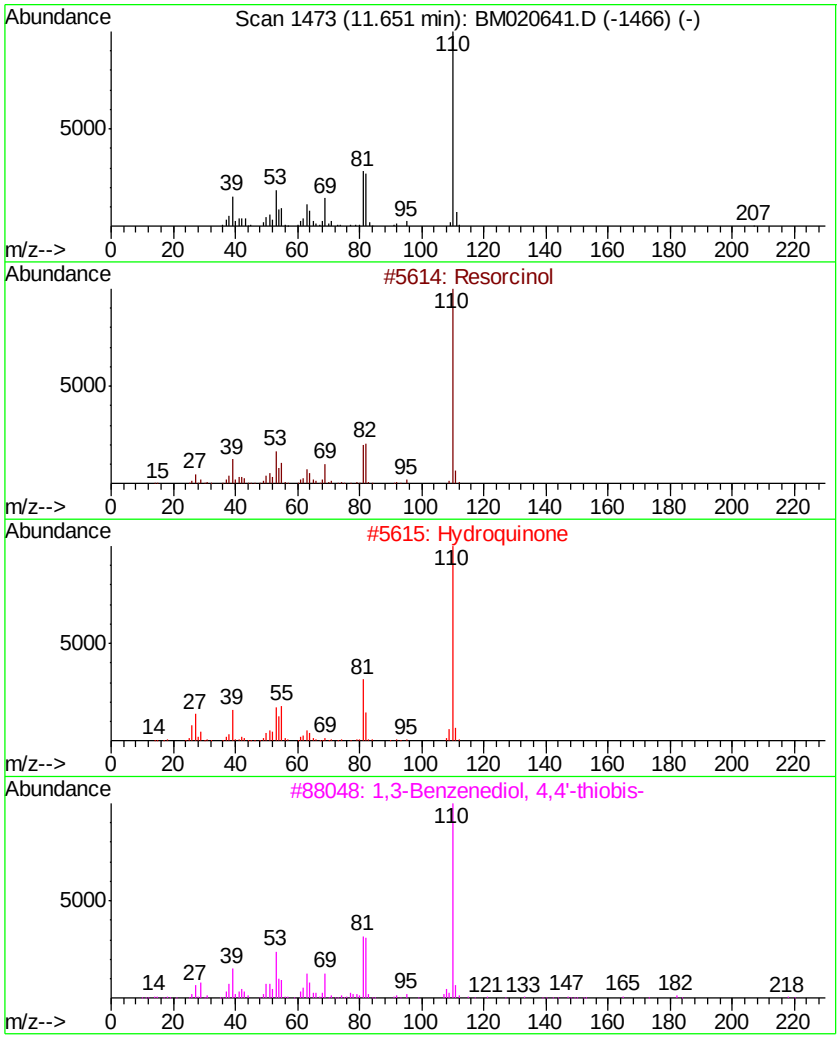
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

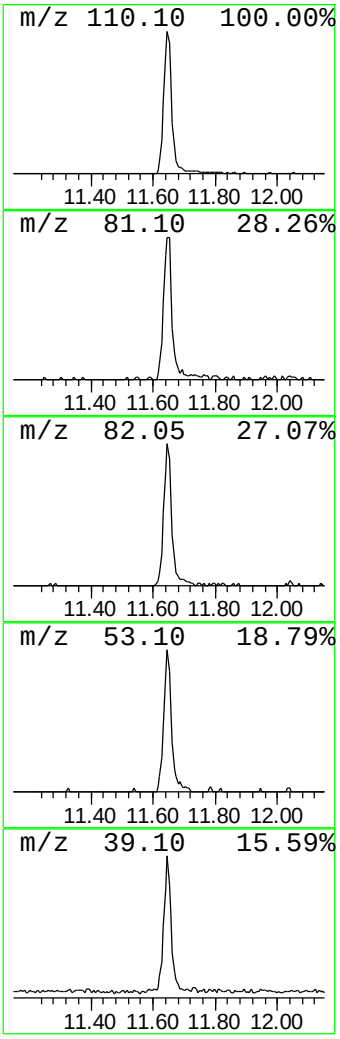
****

Peak Number 4 Resorcinol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	2.59 ng	349905	Naphthalene-d8	10.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Resorcinol	110	C6H6O2	000108-46-3	97
2	Hydroquinone	110	C6H6O2	000123-31-9	72
3	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	64
4	Phenol, 4-ethoxy-	138	C8H10O2	000622-62-8	64
5	3(2H)-Pyridazinone, 6-methyl-	110	C5H6N2O	013327-27-0	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053119\
Data File : BM020641.D
Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

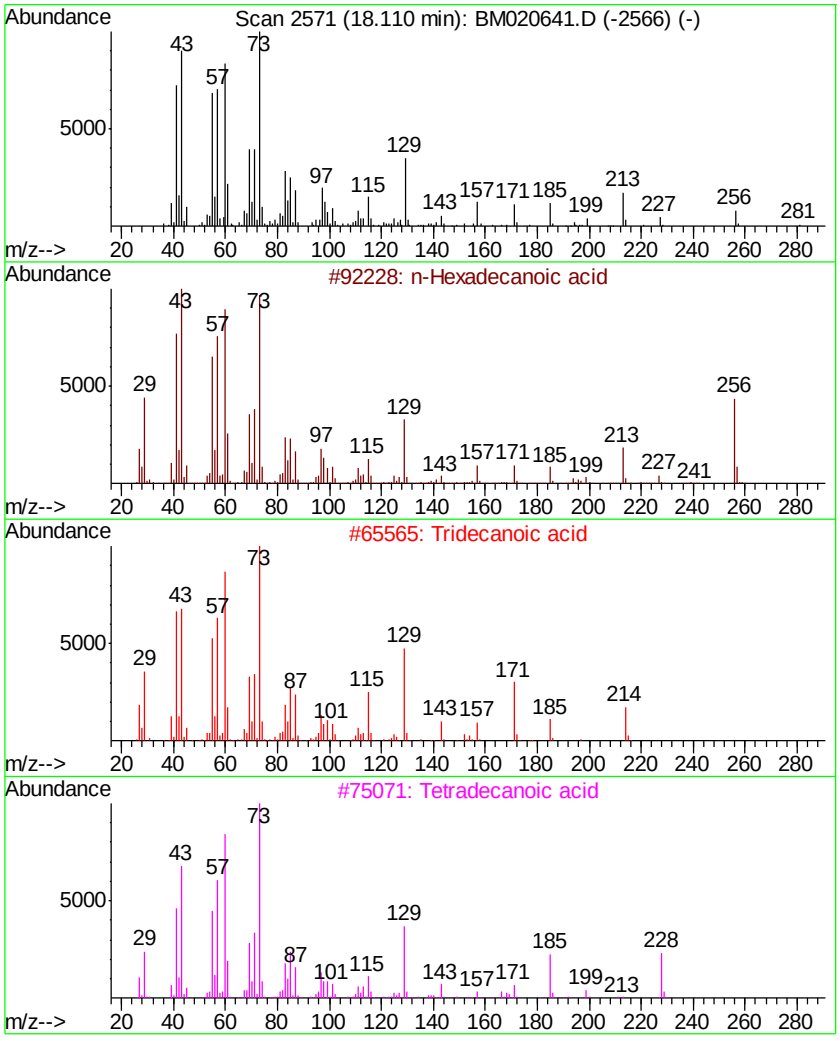
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

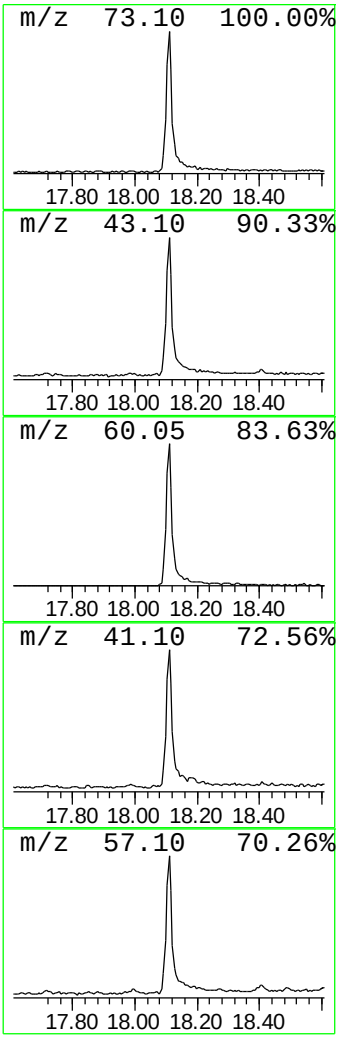
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.11	5.51 ng	797302	Phenanthrene-d10	17.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM053119\
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Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

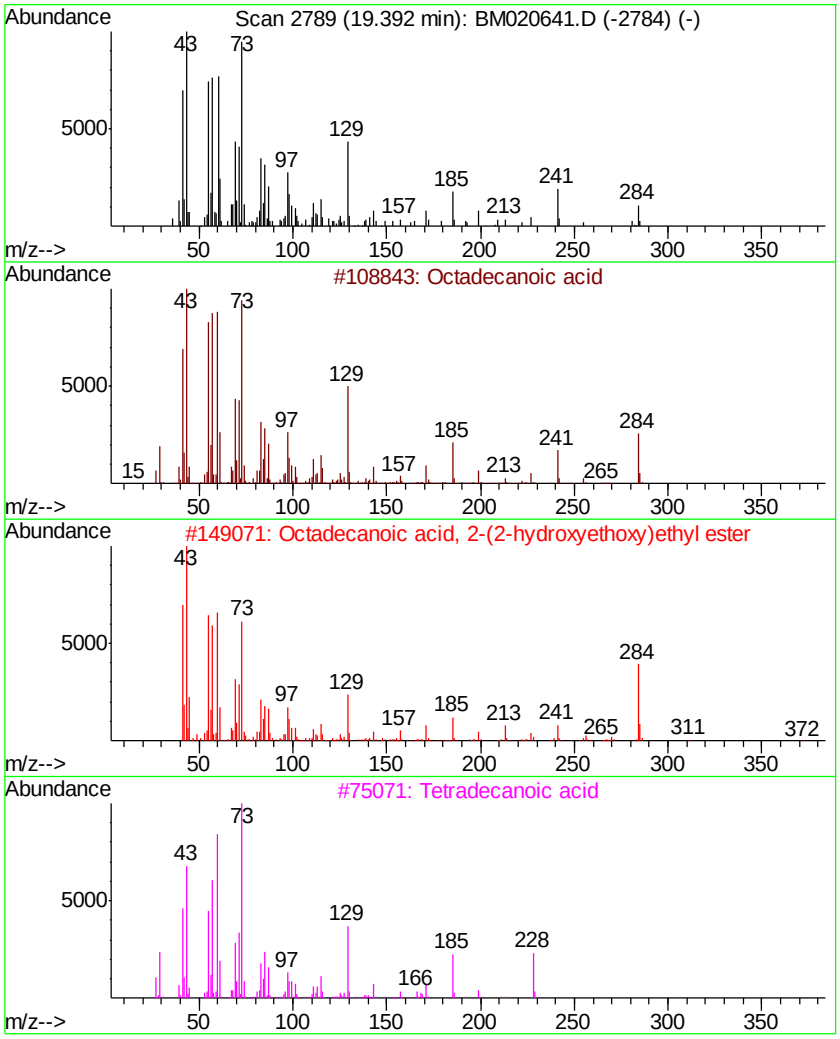
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

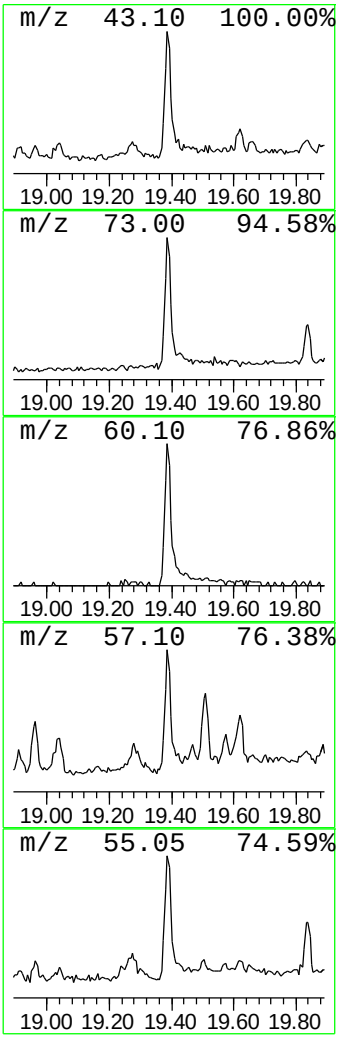
****

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	2.17 ng	311249	Chrysene-d12	21.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Library Search Compound Report

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Data File : BM020641.D
Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

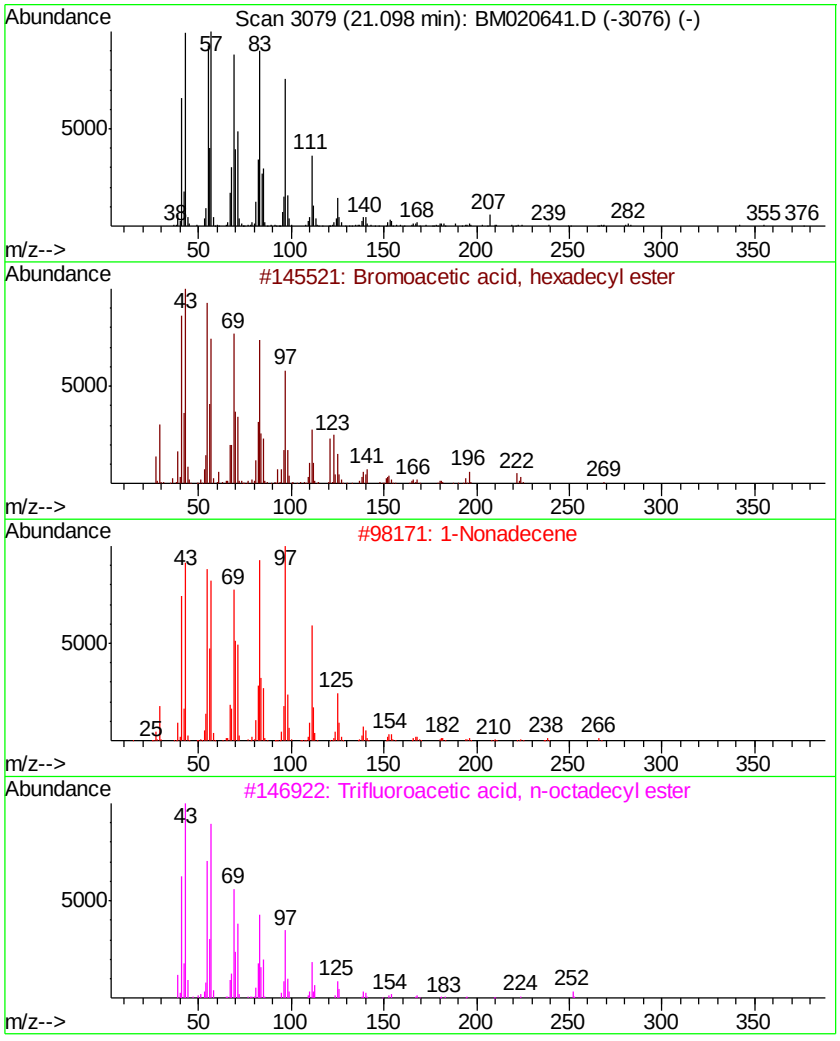
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

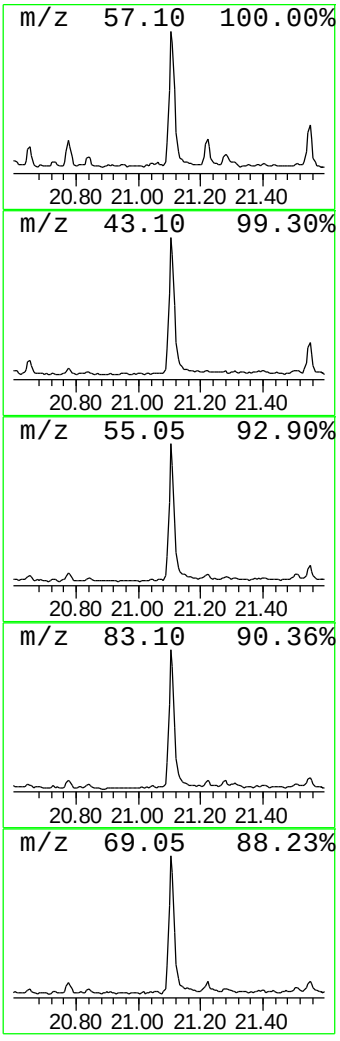
****

Peak Number 7 Bromoacetic acid, hexadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	10.14 ng	1452850	Chrysene-d12	21.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	91
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

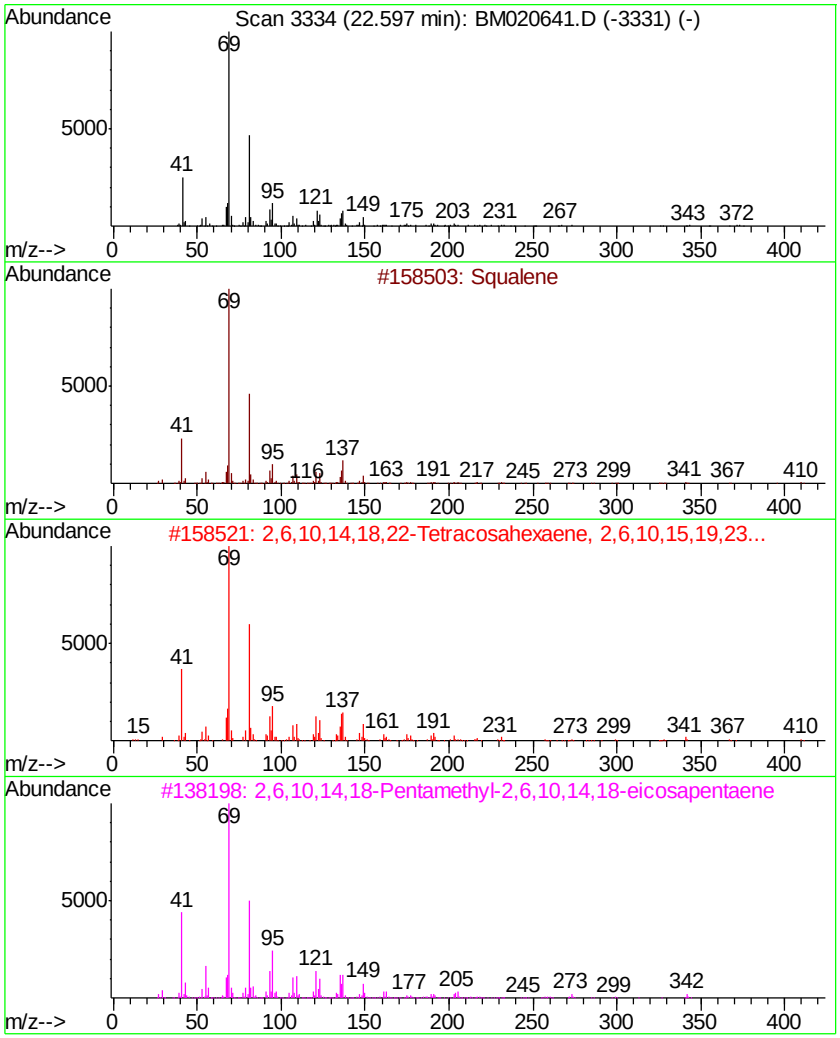
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

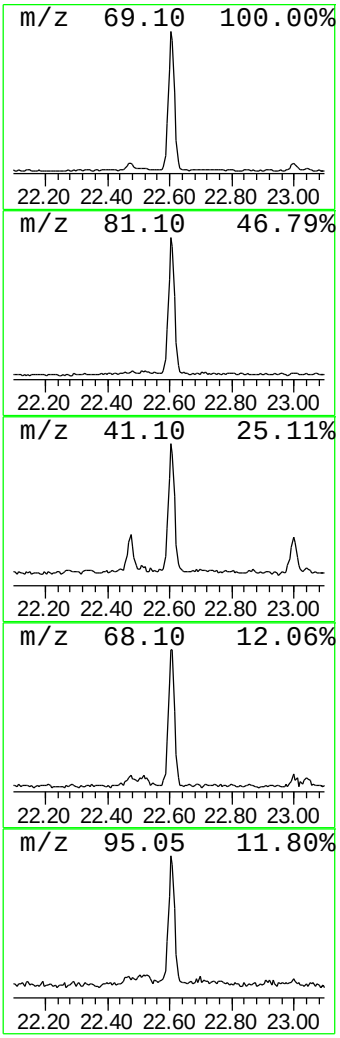
****

Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.60	4.18 ng	647756	Perylene-d12	23.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.M
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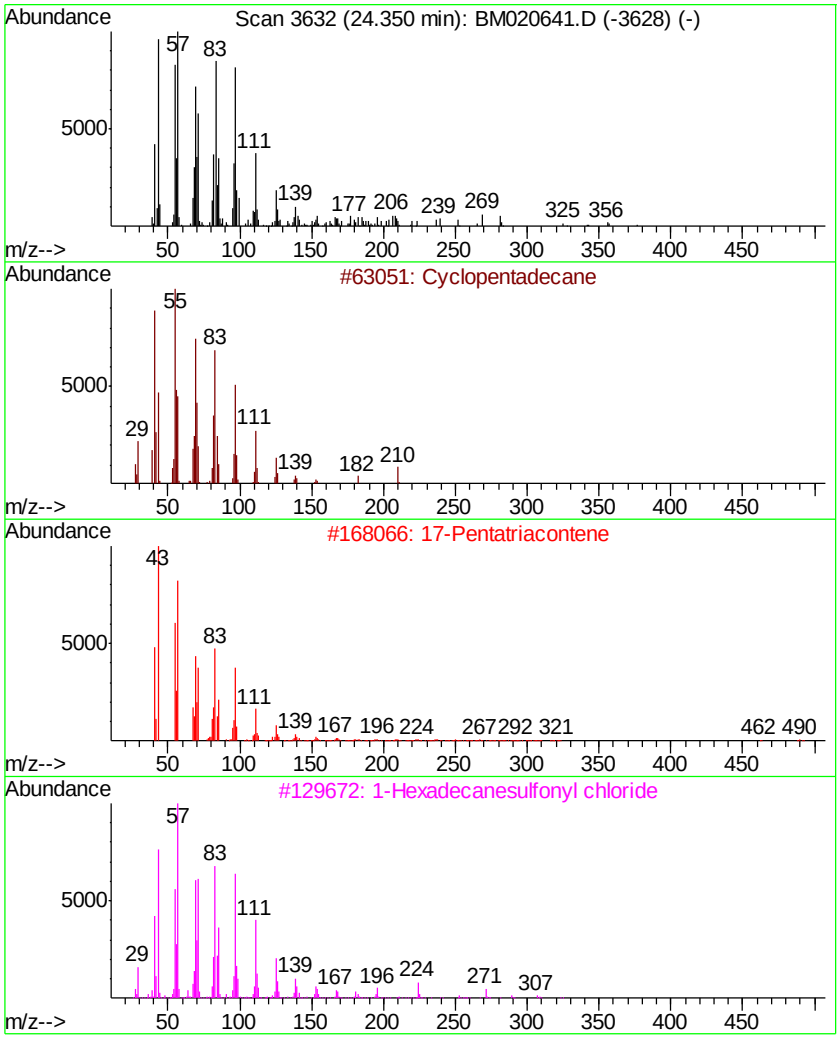
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

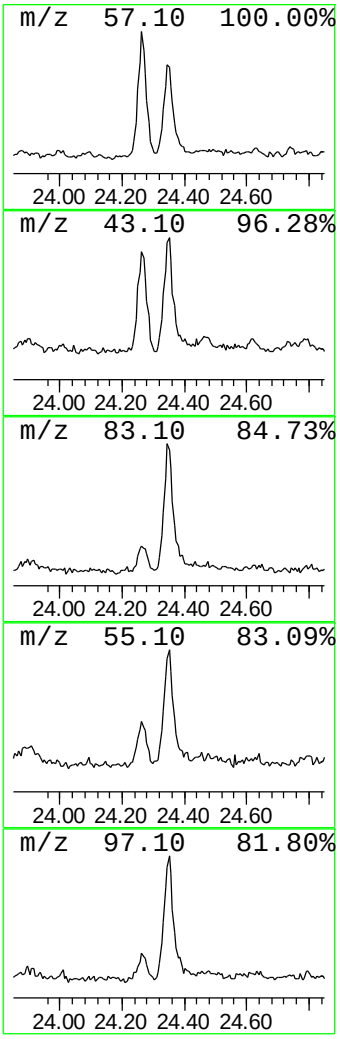
****

Peak Number 9 Cyclopentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.35	2.26 ng	349457	Perylene-d12	23.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	92
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
4	Cyclotetracosane	336	C24H48	000297-03-0	87
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM053119\
Data File : BM020641.D
Acq On : 31 May 2019 22:36
Operator : JU/SJ
Sample : K3072-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM053119.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
Butane, 2-methoxy...	3.07	28.5	ng	2843020	1	7.83	1993690	20.0
unknown7.37	7.37	111.6	ng	11123100	1	7.83	1993690	20.0
Resorcinol	11.65	2.6	ng	349905	2	10.63	2700610	20.0
n-Hexadecanoic acid	18.11	5.5	ng	797302	4	17.22	2892110	20.0
Octadecanoic acid	19.39	2.2	ng	311249	5	21.39	2866770	20.0
Bromoacetic acid,...	21.10	10.1	ng	1452850	5	21.39	2866770	20.0
Squalene	22.60	4.2	ng	647756	6	23.68	3097730	20.0
Cyclopentadecane	24.35	2.3	ng	349457	6	23.68	3097730	20.0