LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM060119\
Data File : BM020653.D
Acq On : 01 Jun 2019 16:44
Operator : HP/JU
Sample : K3072-08
Misc :
ALS Vial : 11 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	3.057	8	12	30	rVB	2172168	2767986	14.90%	2.347%
2	5.416	404	413	425	rBV	6124588	9012118	48.51%	7.640%
3	6.992	671	681	696	rBV	6191584	10406313	56.01%	8.822%
4	7.363	735	744	752	rBV	6461083	10149887	54.63%	8.605%
5	7.828	816	823	830	rBV	1148509	1794829	9.66%	1.522%
6	8.151	870	878	885	rBV	4444300	7312468	39.36%	6.199%
7	8.992	1012	1021	1031	rBV	3761418	6202364	33.39%	5.258%
8	10.622	1290	1298	1306	rVB	1528876	2508769	13.50%	2.127%
9	11.645	1464	1472	1483	rVB	239992	404759	2.18%	0.343%
10	13.086	1710	1717	1724	rBV	8729409	13240970	71.27%	11.226%
11	13.921	1853	1859	1868	rBV	972978	1333501	7.18%	1.131%
12	14.463	1942	1951	1960	rBV2	2188175	3380942	18.20%	2.866%
13	15.957	2197	2205	2222	rBV	7703356	10910983	58.73%	9.250%
14	17.209	2411	2418	2426	rBV2	2934039	4111237	22.13%	3.485%
15	18.109	2565	2571	2580	rBV	1016681	1477803	7.95%	1.253%
16	19.386	2783	2788	2800	rBV	372594	597791	3.22%	0.507%
17	19.839	2858	2865	2870	rBV	14968585	18578255	100.00%	15.750%
18	21.103	3075	3080	3091	rBV	1866490	2347435	12.64%	1.990%
19	21.386	3123	3128	3134	rBV	3170356	4025315	21.67%	3.413%
20	21.544	3152	3155	3161	rVB	268828	303338	1.63%	0.257%
21	21.991	3227	3231	3241	rBV3	281526	495450	2.67%	0.420%
22	22.468	3308	3312	3316	rBV	283384	381532	2.05%	0.323%
23	22.603	3330	3335	3341	rVB	617398	847135	4.56%	0.718%
24	22.991	3397	3401	3406	rBV	258219	376408	2.03%	0.319%
25	23.580	3497	3501	3509	rVB	235324	382791	2.06%	0.325%
26	23.680	3511	3518	3526	rVB	1940814	3762171	20.25%	3.190%
27	24.256	3612	3616	3622	rVB2	175774	316585	1.70%	0.268%
28	24.338	3625	3630	3641	rVB2	248862	524423	2.82%	0.445%

Sum of corrected areas: 117953558

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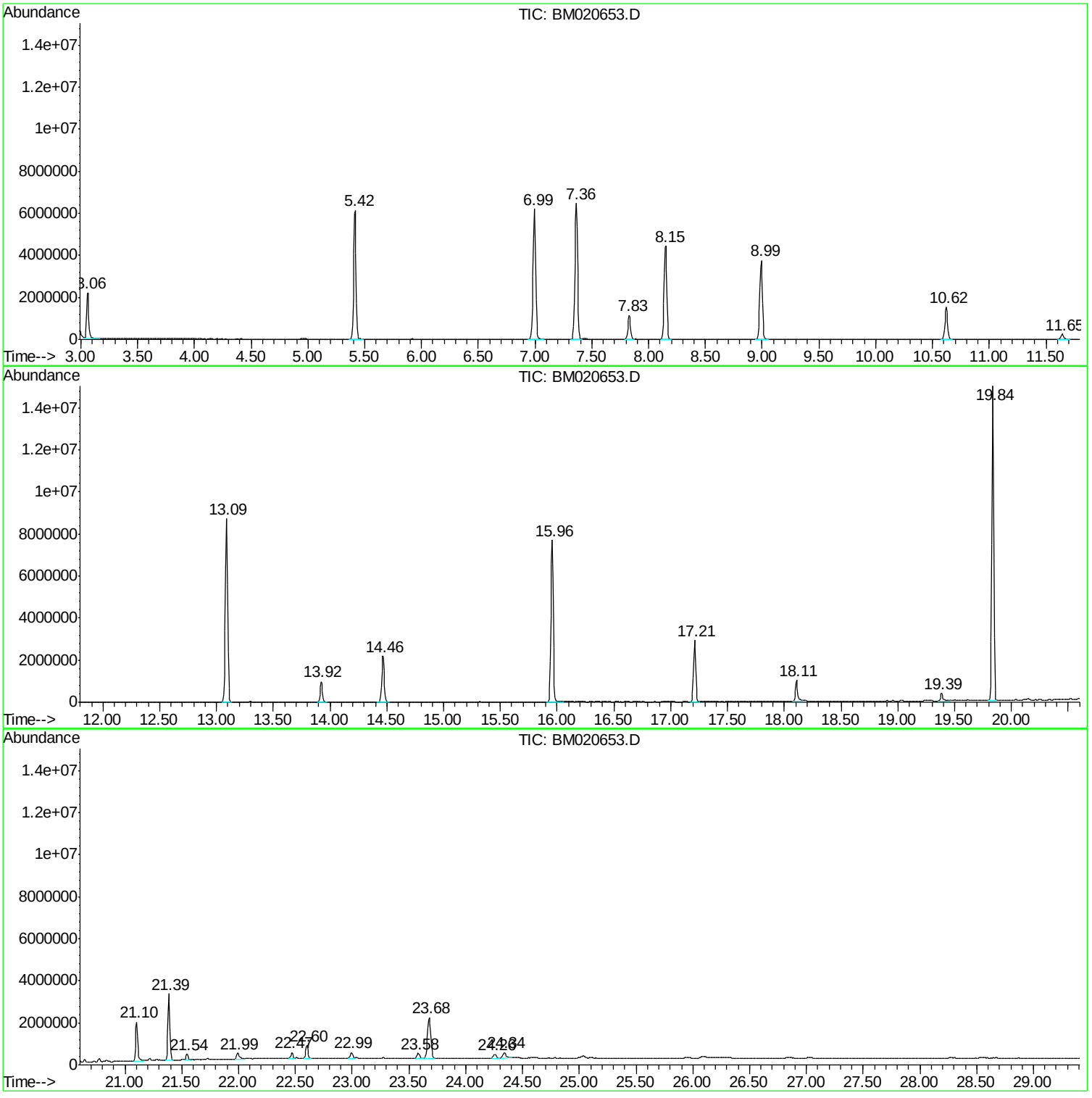
Misc :
ALS Vial : 11 Sample Multiplier: 1

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

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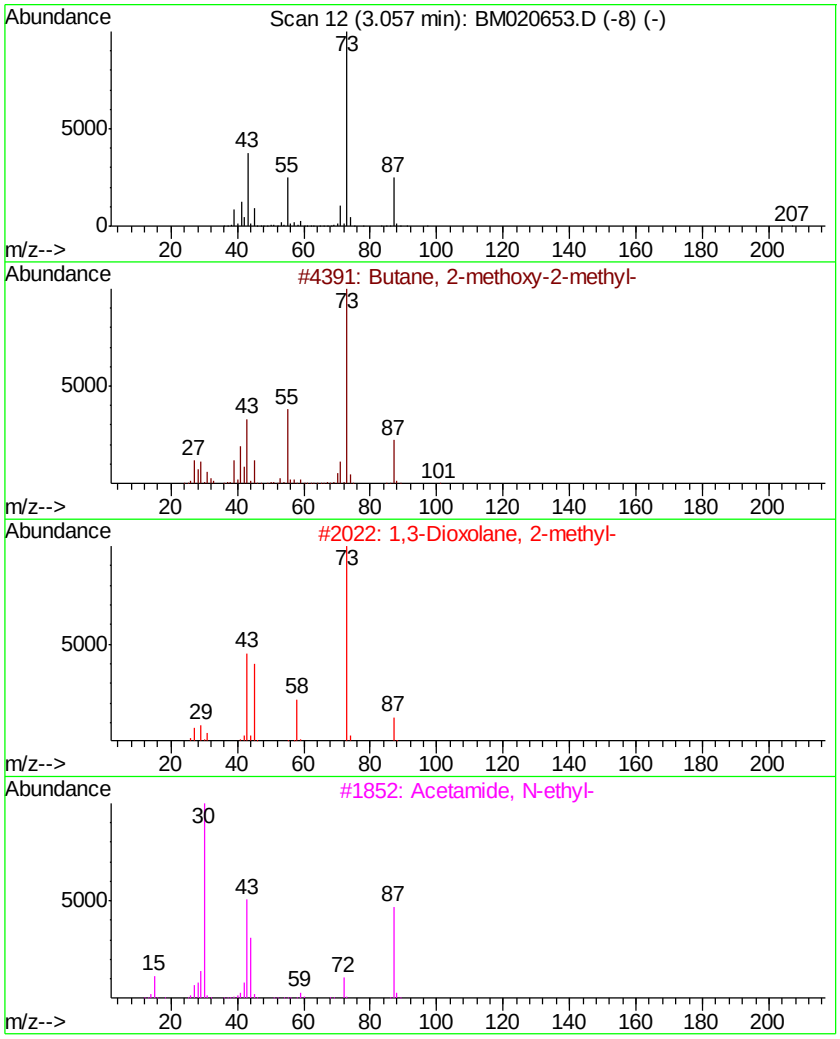
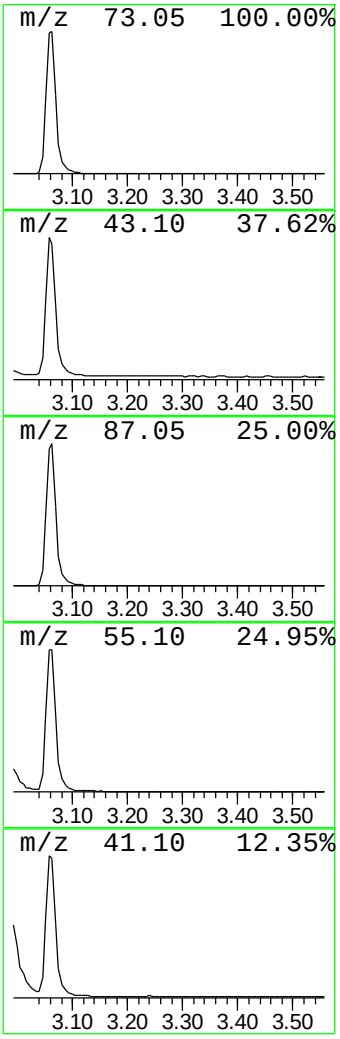
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	30.84 ng	2767990	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	83
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Instrument : BNA_M
ClientSampleId : TP-8

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

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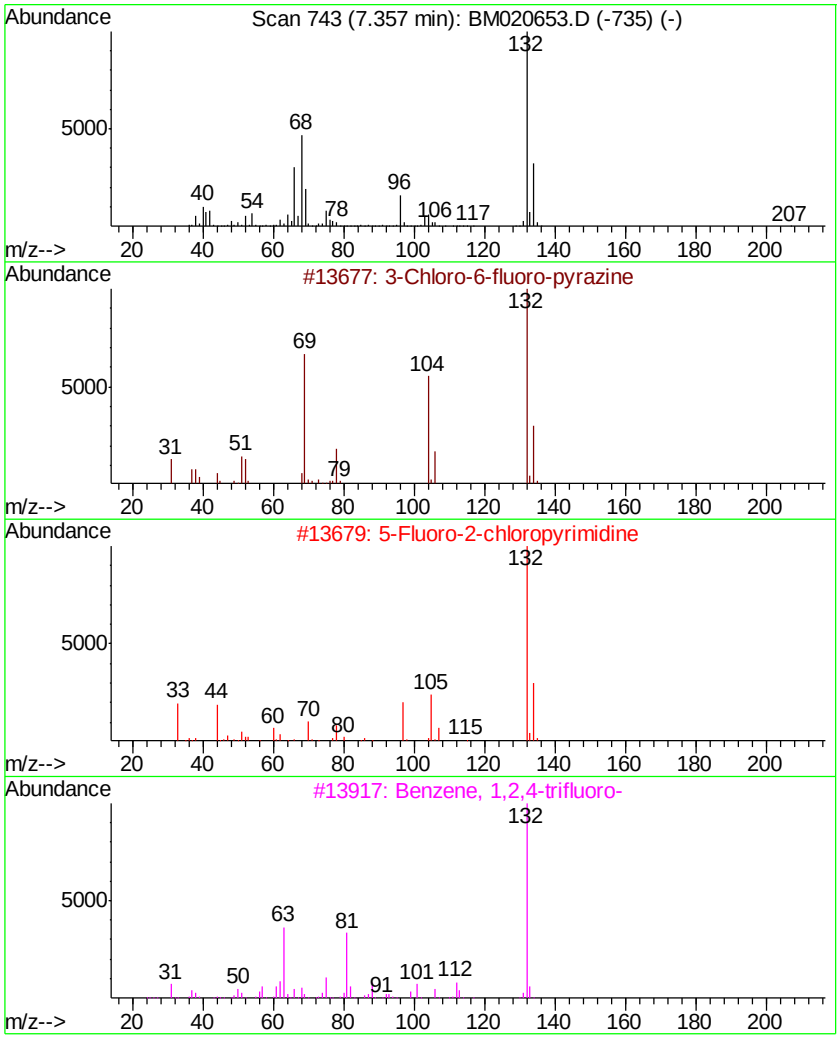
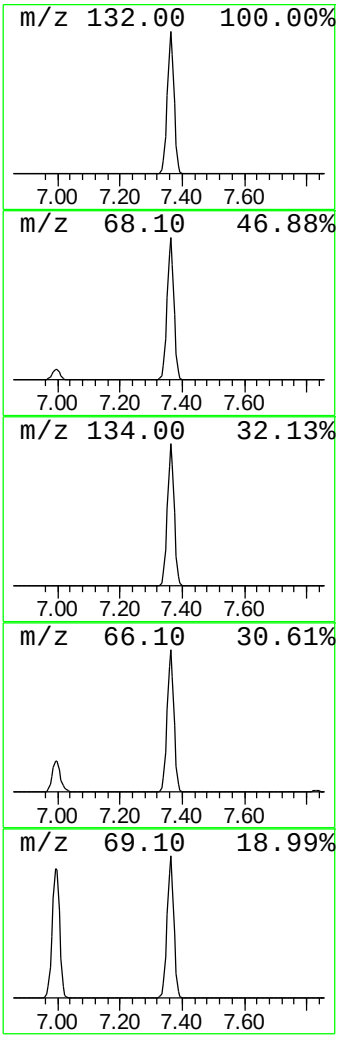
Peak Number 2 unknown7.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	113.10 ng	10149900	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Instrument : BNA_M
ClientSampleId : TP-8

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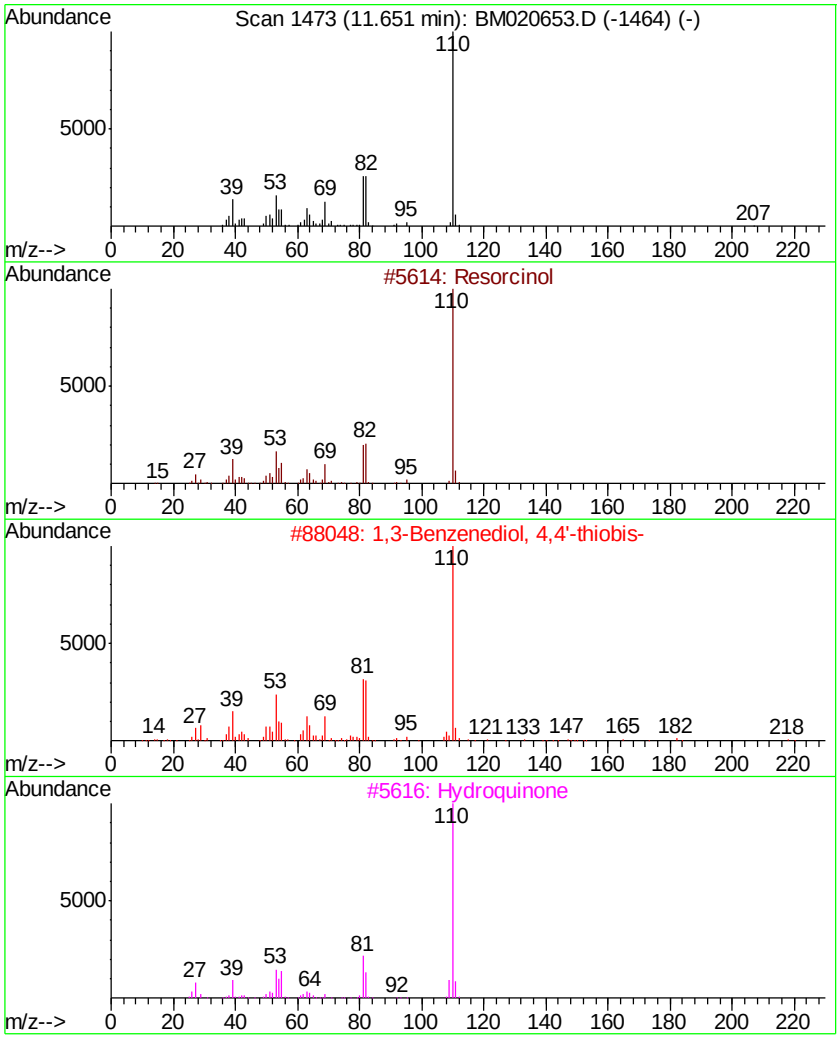
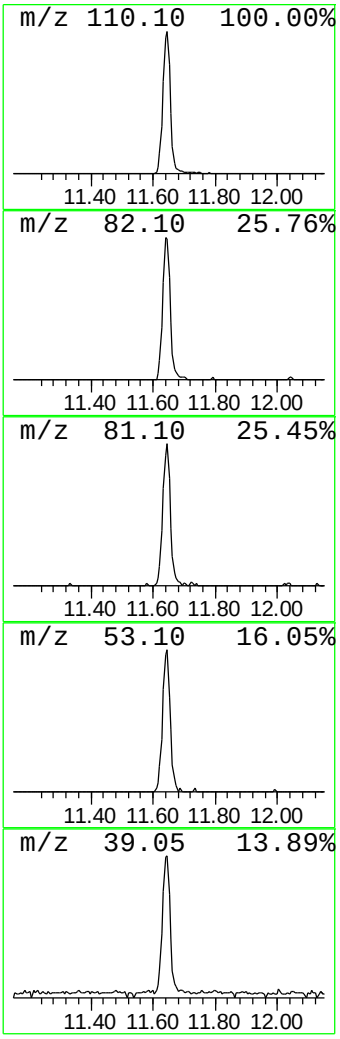
****

Peak Number 4 Resorcinol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	3.23 ng	404759	Naphthalene-d8	10.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Resorcinol	110	C6H6O2	000108-46-3	97
2	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	90
3	Hydroquinone	110	C6H6O2	000123-31-9	72
4	1,2-Benzenediol	110	C6H6O2	000120-80-9	64
5	4(1H)-Pyrimidinone, 6-methyl-	110	C5H6N2O	003524-87-6	59





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TIC Library : C:\DATABASE\NIST02.L
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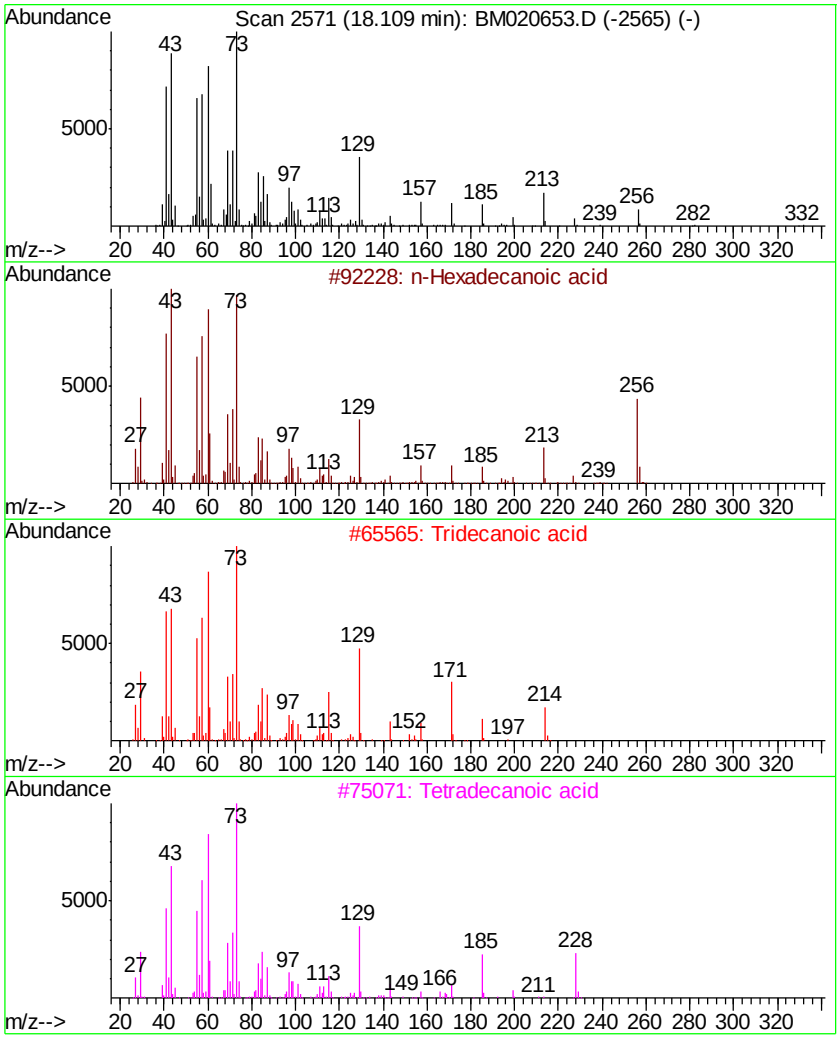
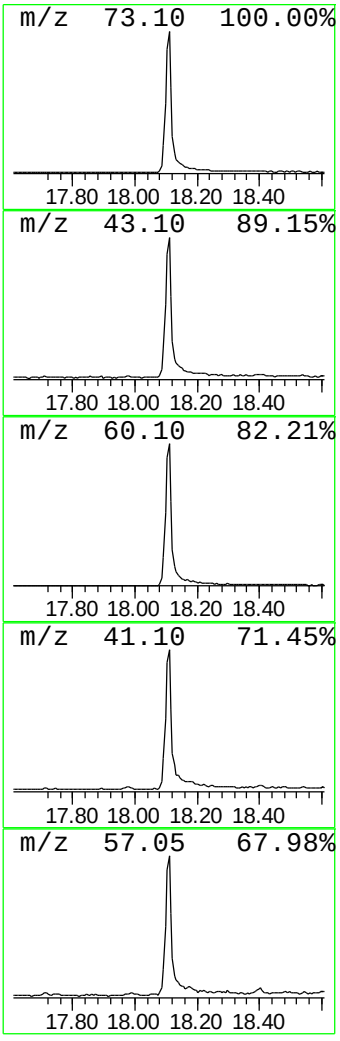
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.11	7.19 ng	1477800	Phenanthrene-d10	17.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	Eicosane	282	C20H42	000112-95-8	25
5	Dodecane	170	C12H26	000112-40-3	11





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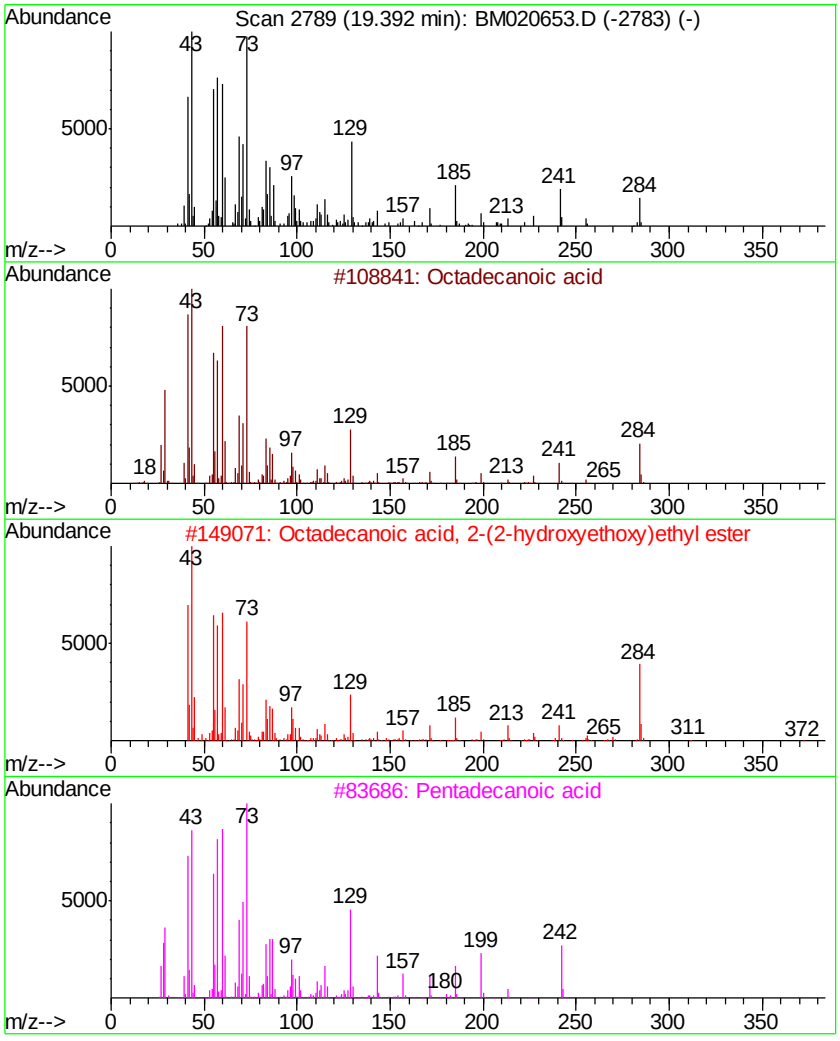
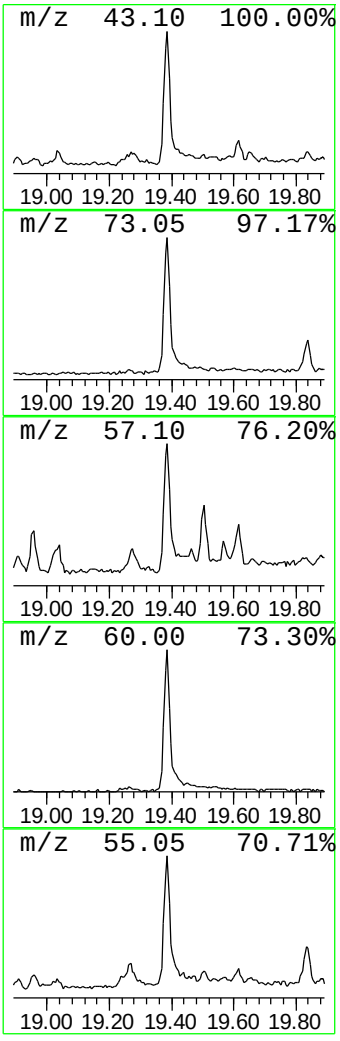
****

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	2.97 ng	597791	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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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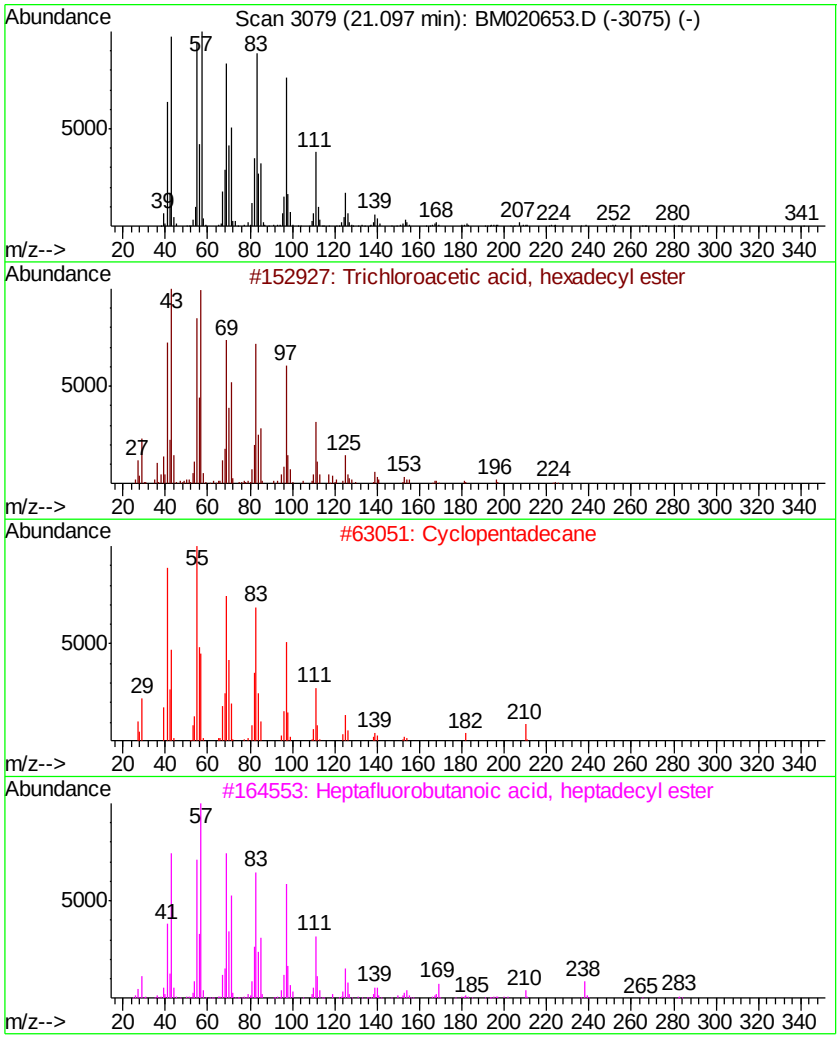
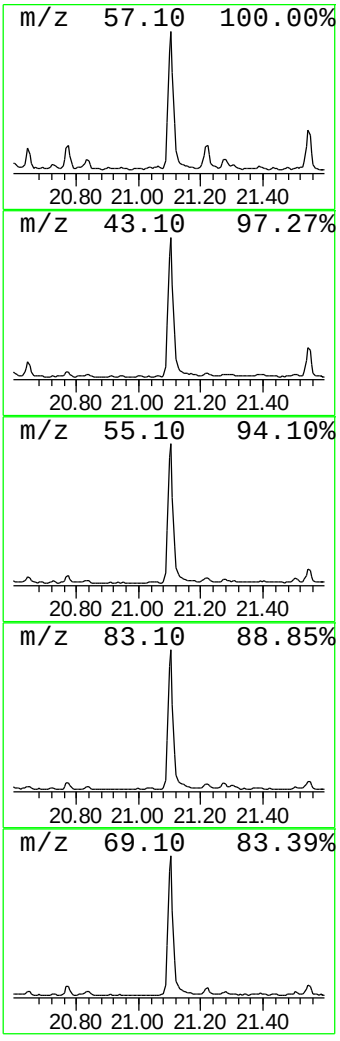
****

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	11.66 ng	2347440	Chrysene-d12	21.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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TIC Library : C:\DATABASE\NIST02.L
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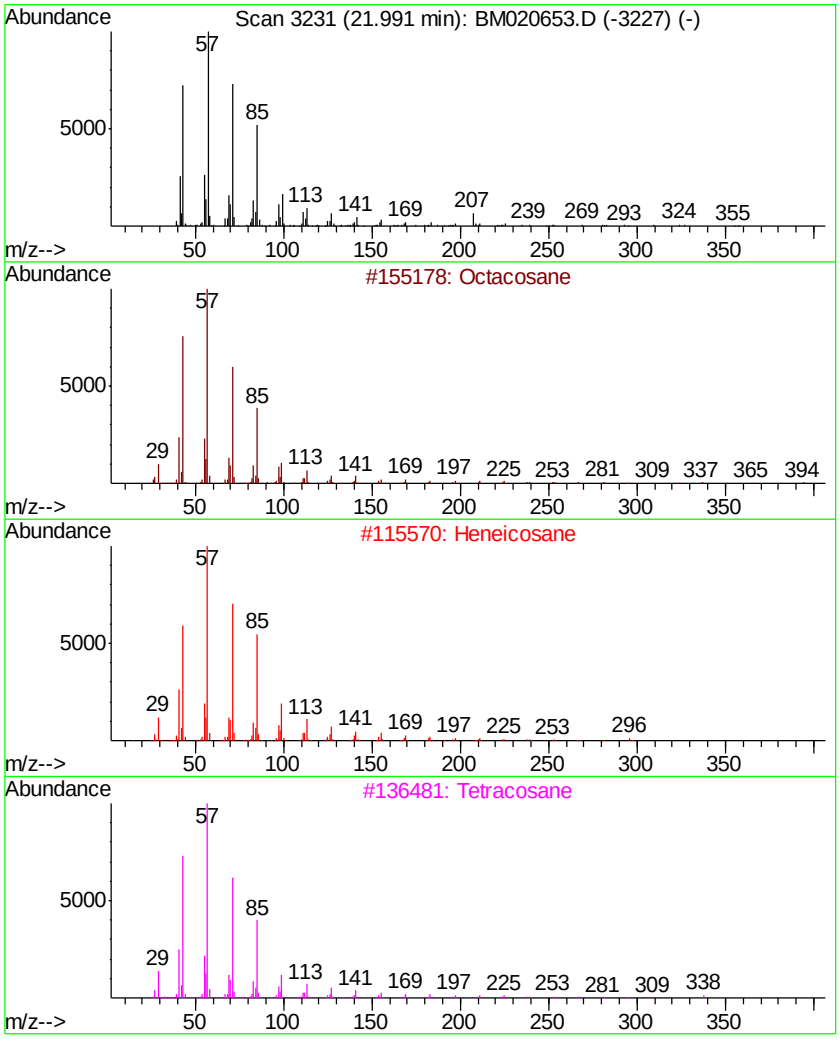
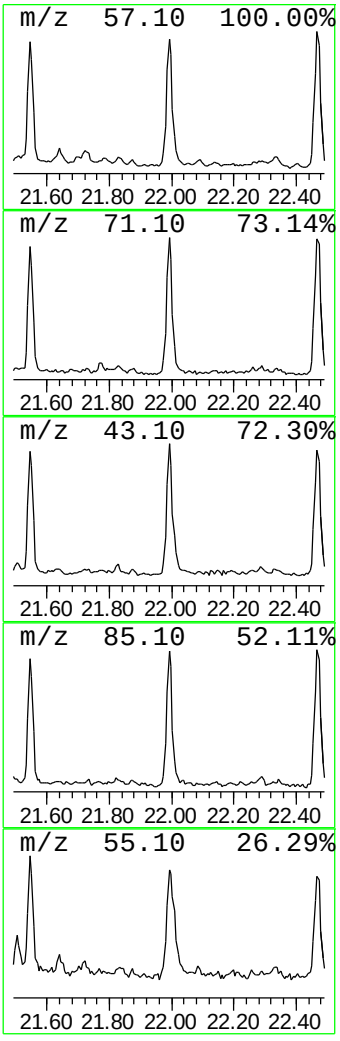
Peak Number 8 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.99	2.46 ng	495450	Chrysene-d12	21.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heptadecane	240	C17H36	000629-78-7	91





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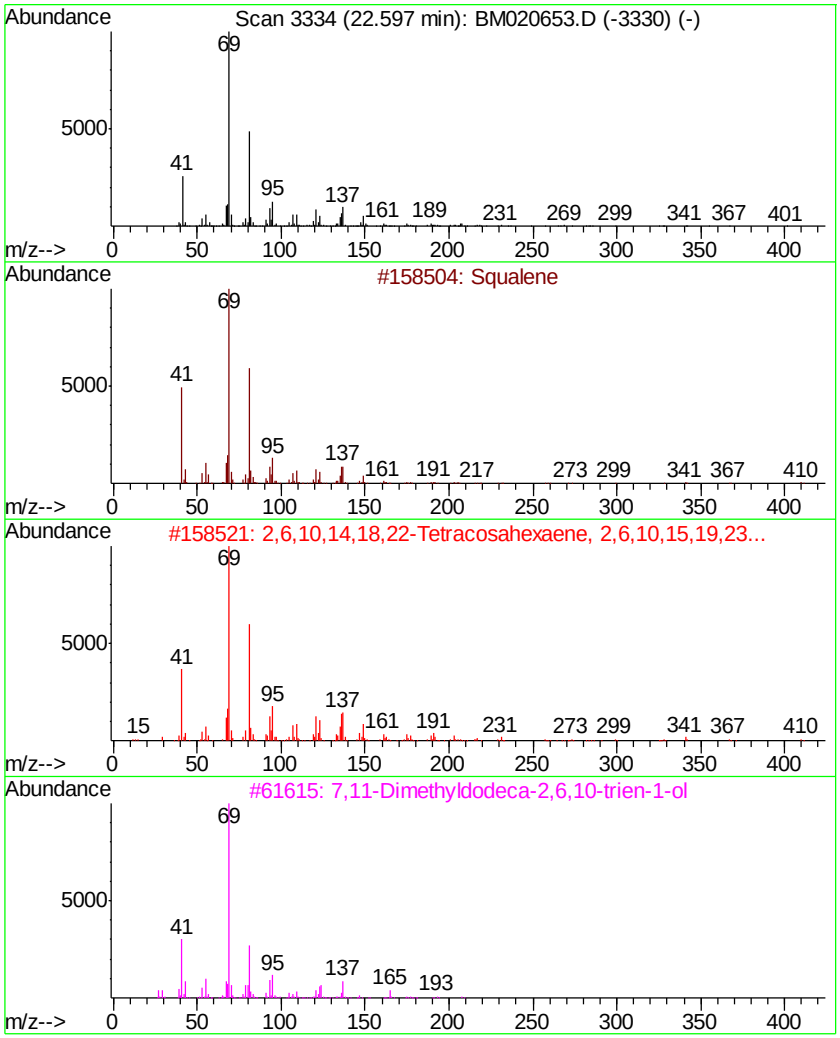
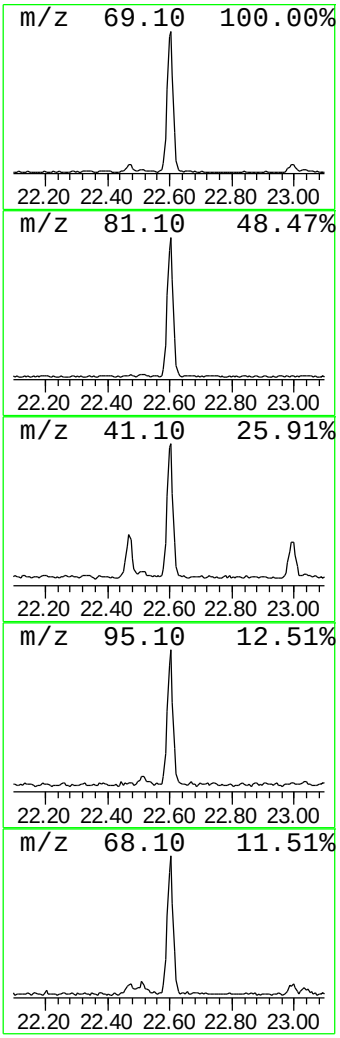
Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.60	4.50 ng	847135	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	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
5	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72





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TIC Library : C:\DATABASE\NIST02.L
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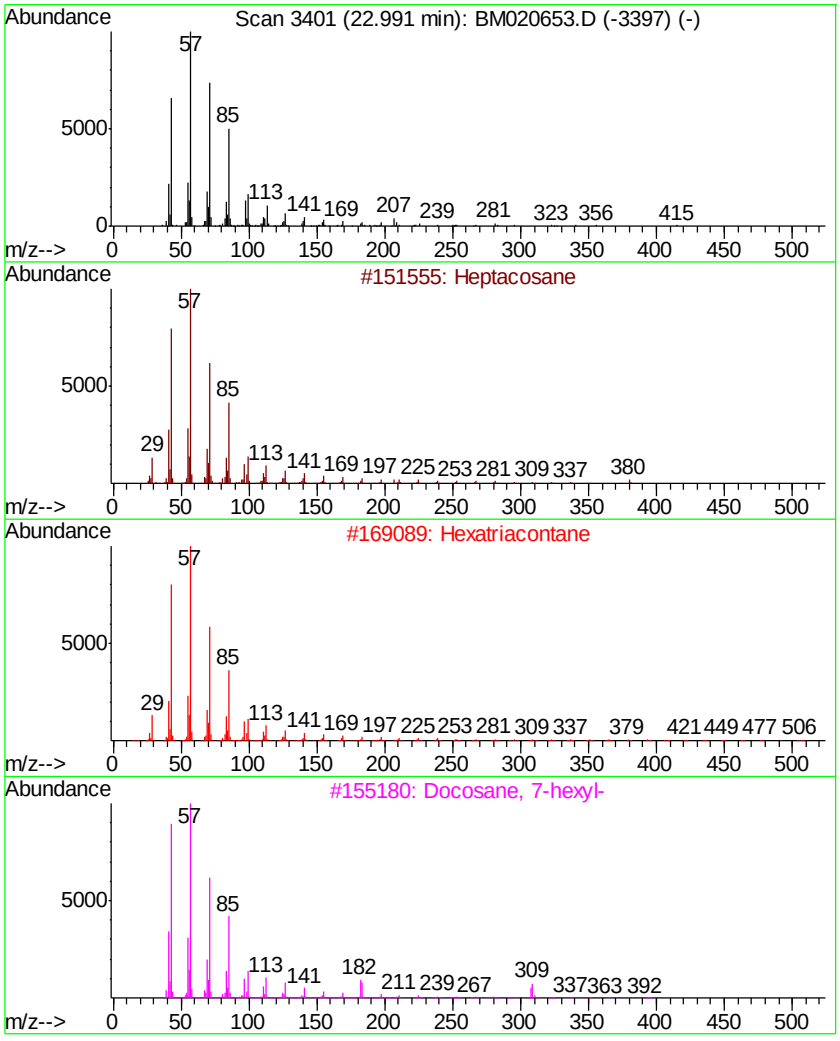
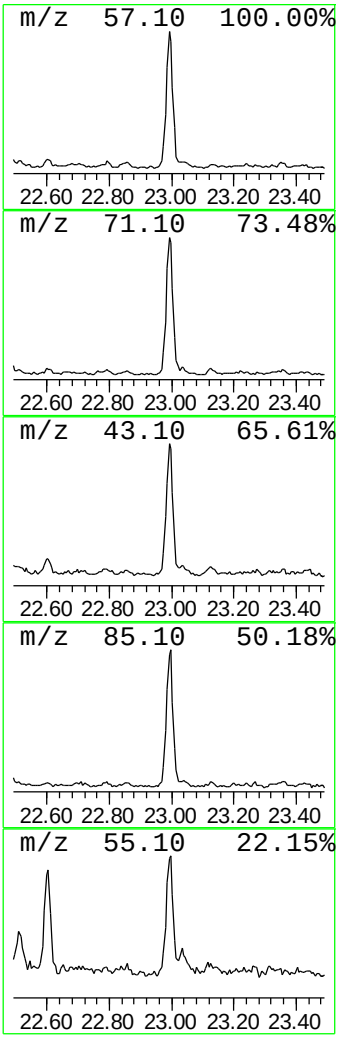
Peak Number 10 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.99	2.00 ng	376408	Perylene-d12	23.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Hexatriacontane	507	C36H74	000630-06-8	91
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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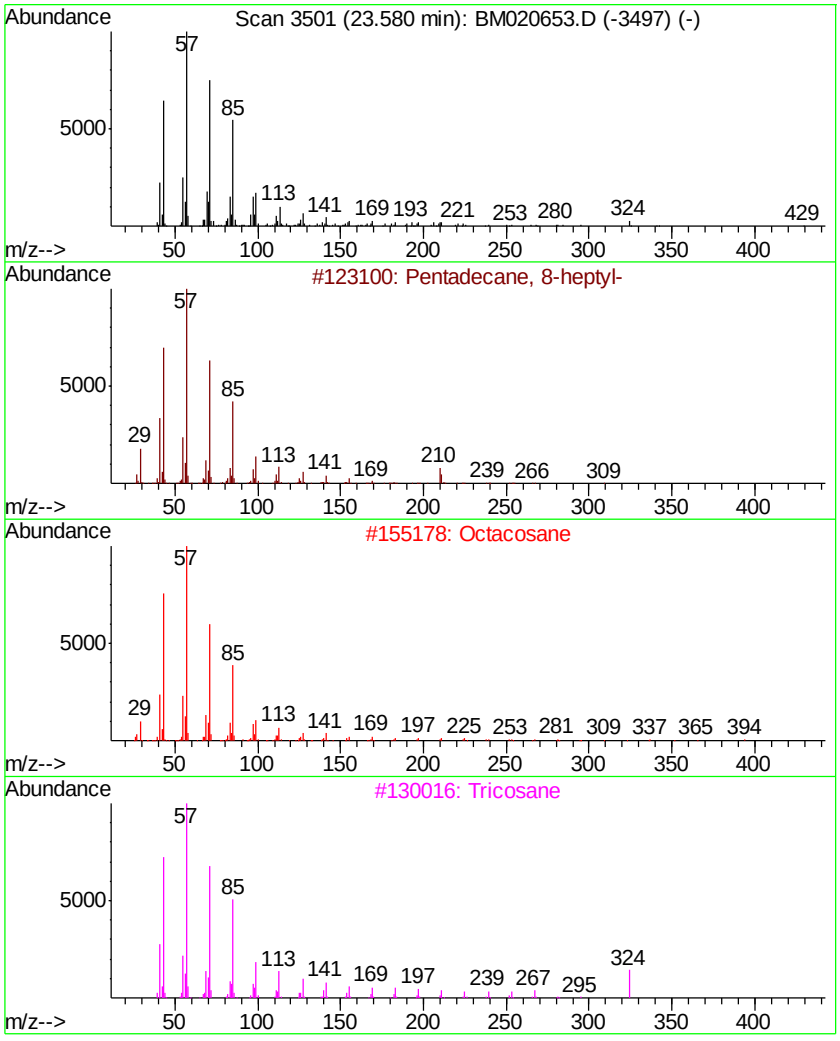
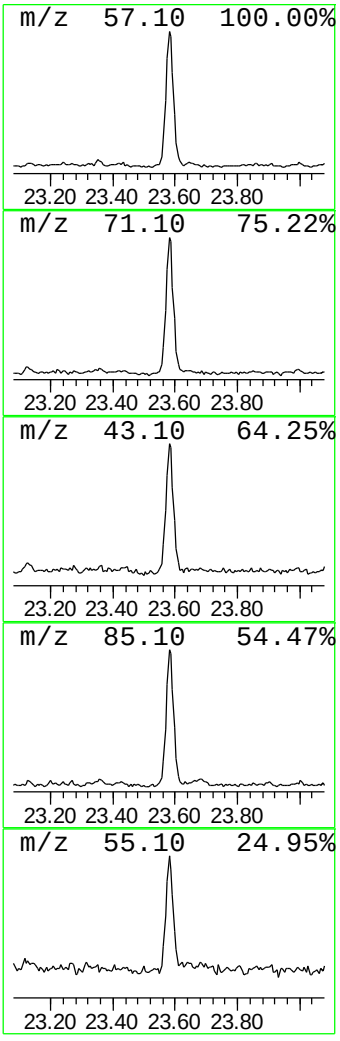
Peak Number 11 Pentadecane, 8-heptyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	2.03 ng	382791	Perylene-d12	23.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tricosane	324	C23H48	000638-67-5	90
4	Nonacosane	408	C29H60	000630-03-5	90
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM060119\
Data File : BM020653.D
Acq On : 01 Jun 2019 16:44
Operator : HP/JU
Sample : K3072-08
Misc :
ALS Vial : 11 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

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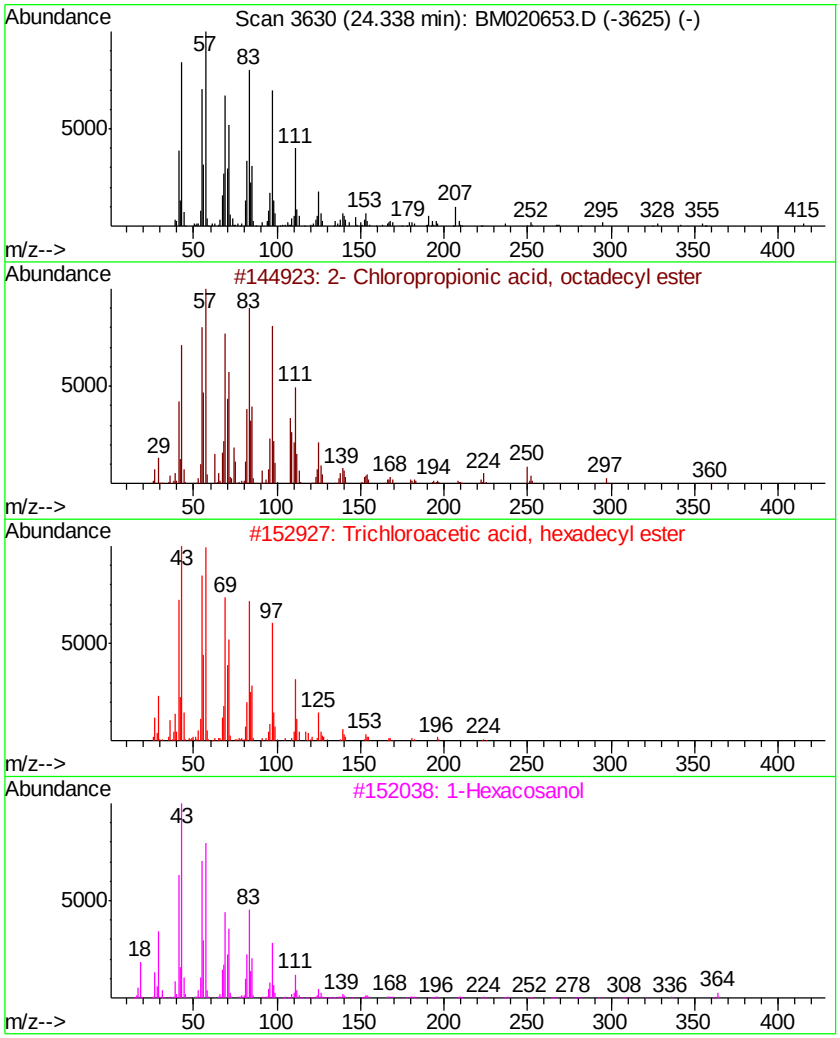
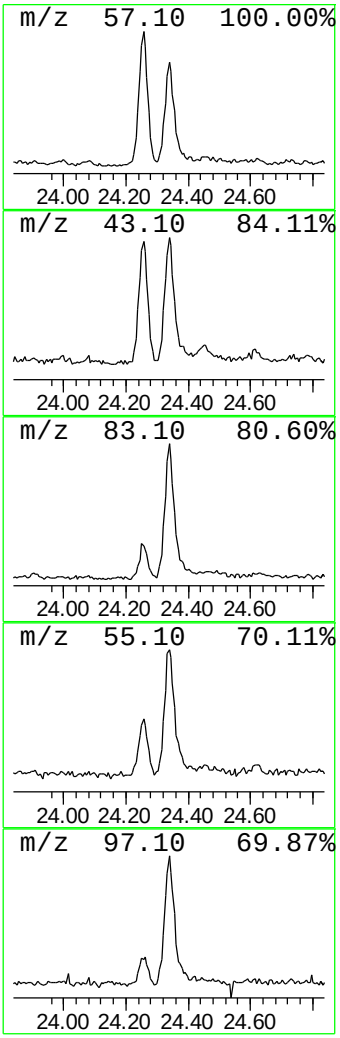
Peak Number 12 2- Chloropropionic acid, oc... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.34	2.79 ng	524423	Perylene-d12	23.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	1-Hexacosanol	382	C26H54O	000506-52-5	87
4	1-Tetracosanol	354	C24H50O	000506-51-4	87
5	1-Octadecene	252	C18H36	000112-88-9	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM060119\
Data File : BM020653.D
Acq On : 01 Jun 2019 16:44
Operator : HP/JU
Sample : K3072-08
Misc :
ALS Vial : 11 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...	3.06	30.8	ng	2767990	1	7.83	1794830	20.0
unknown7.36	7.36	113.1	ng	10149900	1	7.83	1794830	20.0
Resorcinol	11.65	3.2	ng	404759	2	10.62	2508770	20.0
n-Hexadecanoic acid	18.11	7.2	ng	1477800	4	17.21	4111240	20.0
Octadecanoic acid	19.39	3.0	ng	597791	5	21.39	4025320	20.0
Trichloroacetic a...	21.10	11.7	ng	2347440	5	21.39	4025320	20.0
Octacosane	21.99	2.5	ng	495450	5	21.39	4025320	20.0
Squalene	22.60	4.5	ng	847135	6	23.68	3762170	20.0
Heptacosane	22.99	2.0	ng	376408	6	23.68	3762170	20.0
Pentadecane, 8-he...	23.58	2.0	ng	382791	6	23.68	3762170	20.0
2- Chloropropioni...	24.34	2.8	ng	524423	6	23.68	3762170	20.0