LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016269.D
Acq On : 09 Aug 2018 04:39
Operator : SJ/JU
Sample : J4328-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-24

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-BM072318.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	5.187	317	323	330	rBV	45198	71763	2.15%	0.377%
2	5.381	347	356	371	rBV	2290816	3334815	100.00%	17.510%
3	5.664	398	404	416	rBV	390585	636429	19.08%	3.342%
4	7.299	676	682	693	rBV	222712	393155	11.79%	2.064%
5	7.657	737	743	755	rBV	839223	1415664	42.45%	7.433%
6	8.128	817	823	836	rBV	193485	363109	10.89%	1.907%
7	8.452	871	878	884	rBV	824710	1345928	40.36%	7.067%
8	8.493	884	885	892	rVB	58260	68269	2.05%	0.358%
9	9.316	1018	1025	1038	rBV	616420	1051962	31.54%	5.524%
10	9.751	1093	1099	1106	rBV	41858	65952	1.98%	0.346%
11	10.869	1283	1289	1297	rBV2	50876	117585	3.53%	0.617%
12	10.946	1297	1302	1315	rVB	225806	390817	11.72%	2.052%
13	13.387	1707	1717	1724	rBV	1454889	2038631	61.13%	10.704%
14	14.086	1831	1836	1849	rBV10	22156	66166	1.98%	0.347%
15	14.581	1917	1920	1928	rVB6	21407	42326	1.27%	0.222%
16	14.769	1945	1952	1957	rBV2	281974	450911	13.52%	2.368%
17	14.834	1957	1963	1972	rVV3	55736	132706	3.98%	0.697%
18	15.163	2016	2019	2026	rVB2	33186	51102	1.53%	0.268%
19	15.745	2114	2118	2122	rVB	33490	46363	1.39%	0.243%
20	15.804	2122	2128	2133	rBV4	36246	84280	2.53%	0.443%
21	16.257	2198	2205	2216	rBV	1233147	1781871	53.43%	9.356%
22	16.480	2238	2243	2250	rBV2	51686	99369	2.98%	0.522%
23	17.304	2378	2383	2389	rVB3	19944	39301	1.18%	0.206%
24	17.504	2411	2417	2422	rBV	337619	498376	14.94%	2.617%
25	18.357	2556	2562	2566	rBV4	77651	124933	3.75%	0.656%
26	19.610	2772	2775	2780	rBV5	40722	61022	1.83%	0.320%
27	20.080	2850	2855	2861	rBV	2402860	3000674	89.98%	15.756%
28	20.839	2981	2984	2988	rBV	32957	37683	1.13%	0.198%
29	21.304	3060	3063	3070	rVB4	60934	79630	2.39%	0.418%
30	21.633	3114	3119	3125	rBV	454660	571914	17.15%	3.003%
31	23.968	3510	3516	3524	rVB	300983	582458	17.47%	3.058%

Sum of corrected areas: 19045164

LSC Report - Integrated Chromatogram

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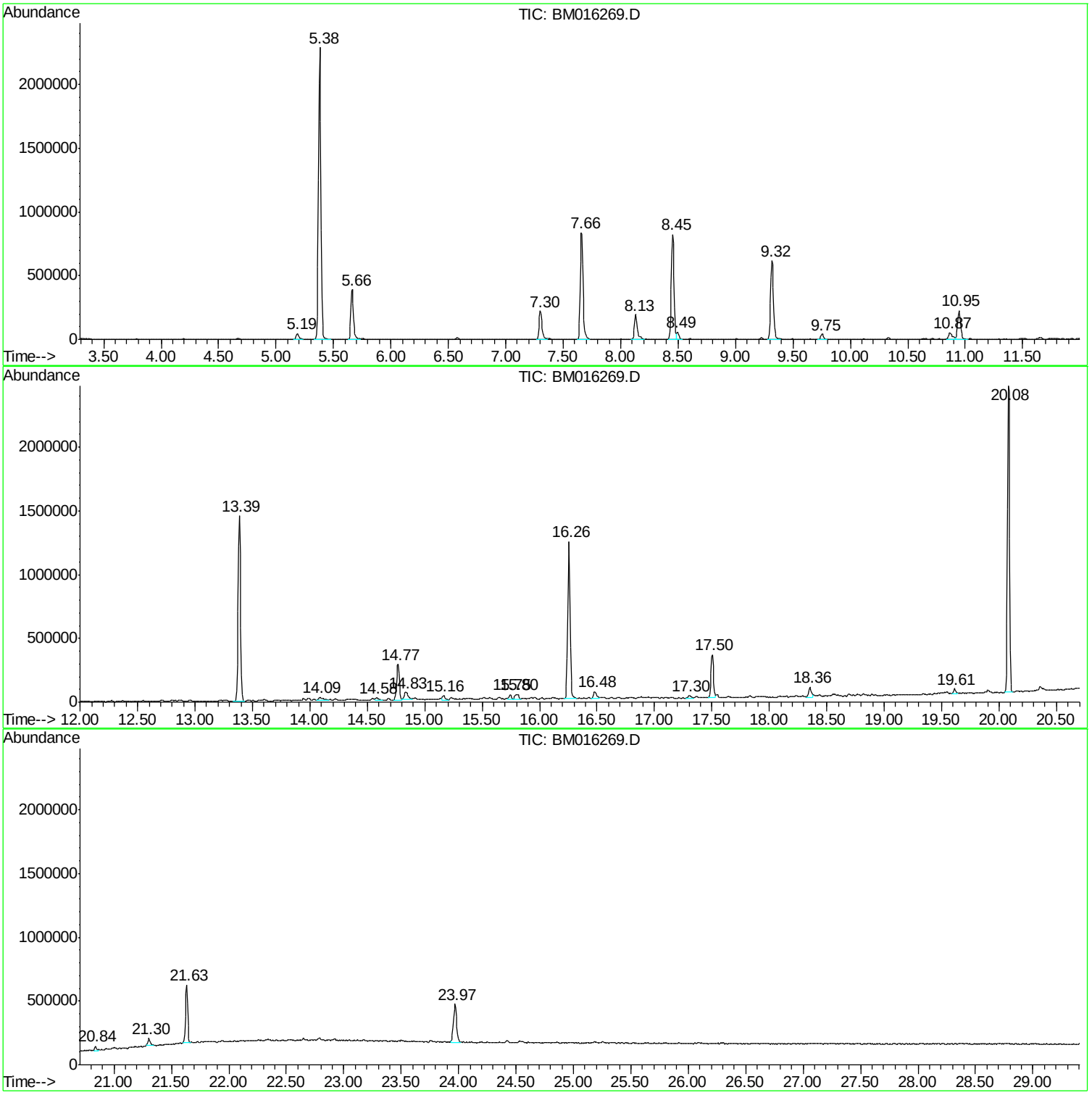
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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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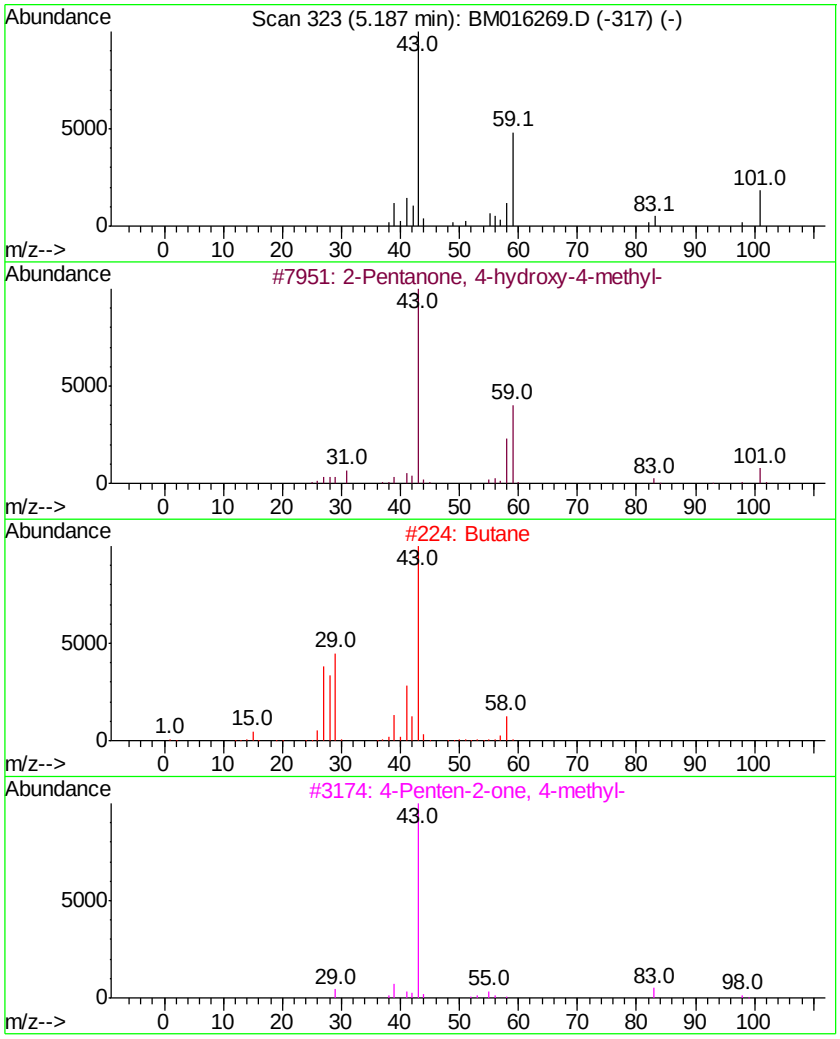
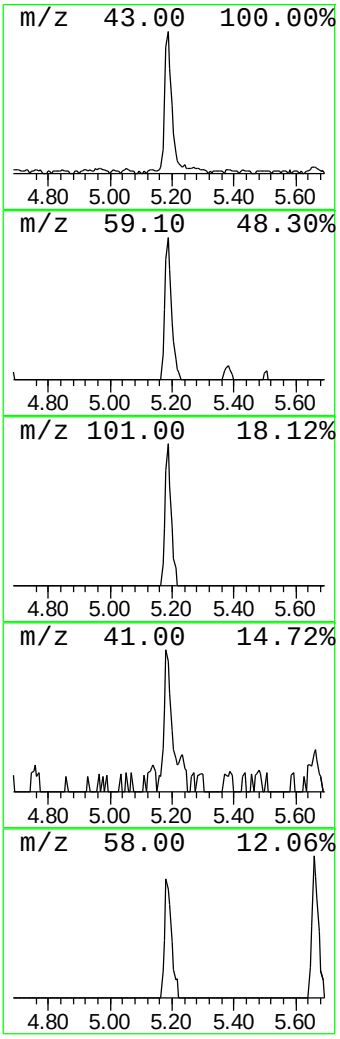
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.95 ng	71763	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Butane	58	C4H10	000106-97-8	22
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Misc :
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Instrument : BNA_M
ClientSampleId : MW-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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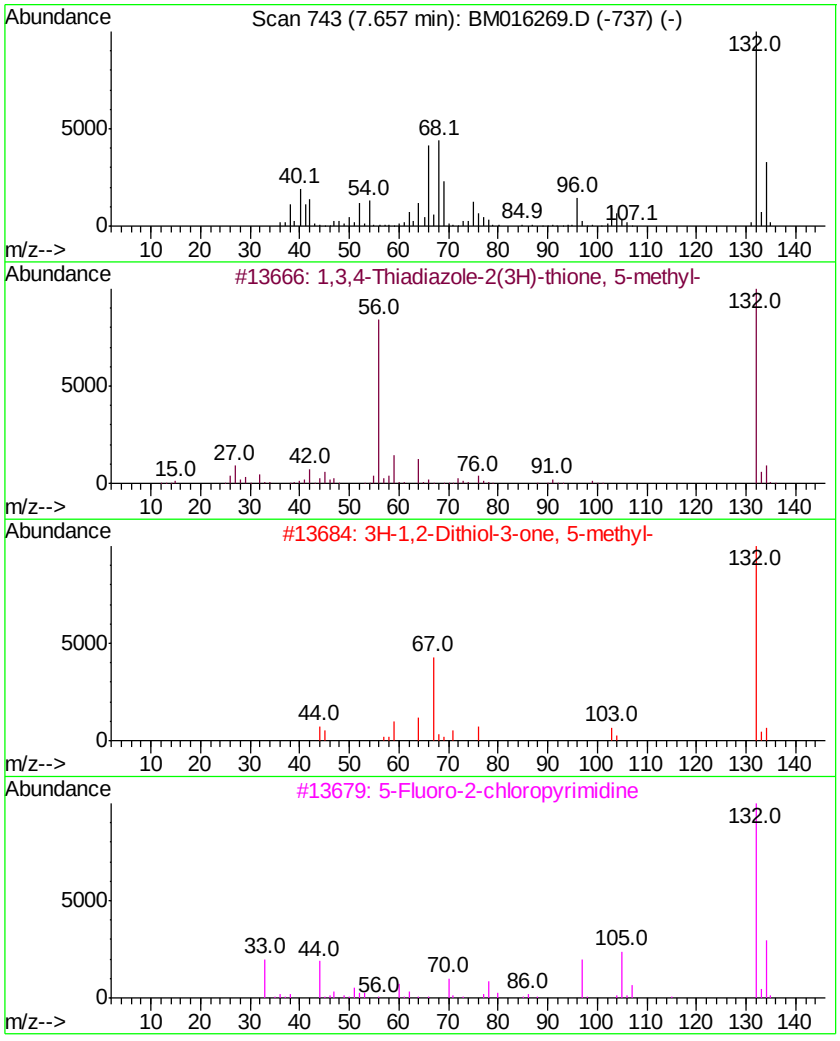
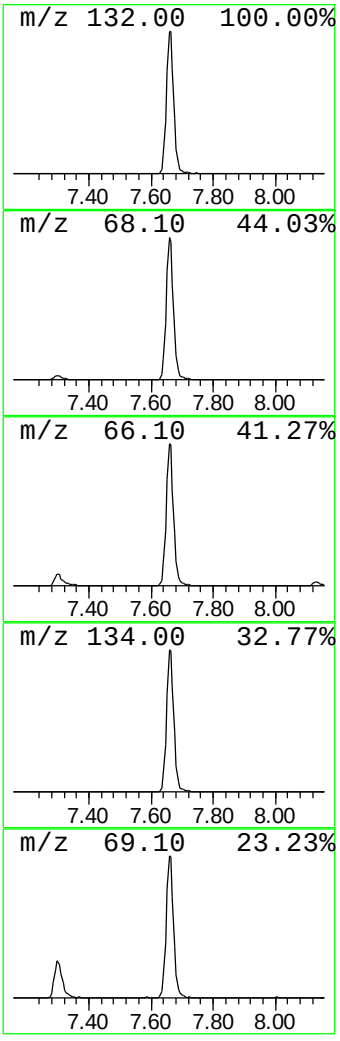
Peak Number 3 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	77.97 ng	1415660	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	14





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-24

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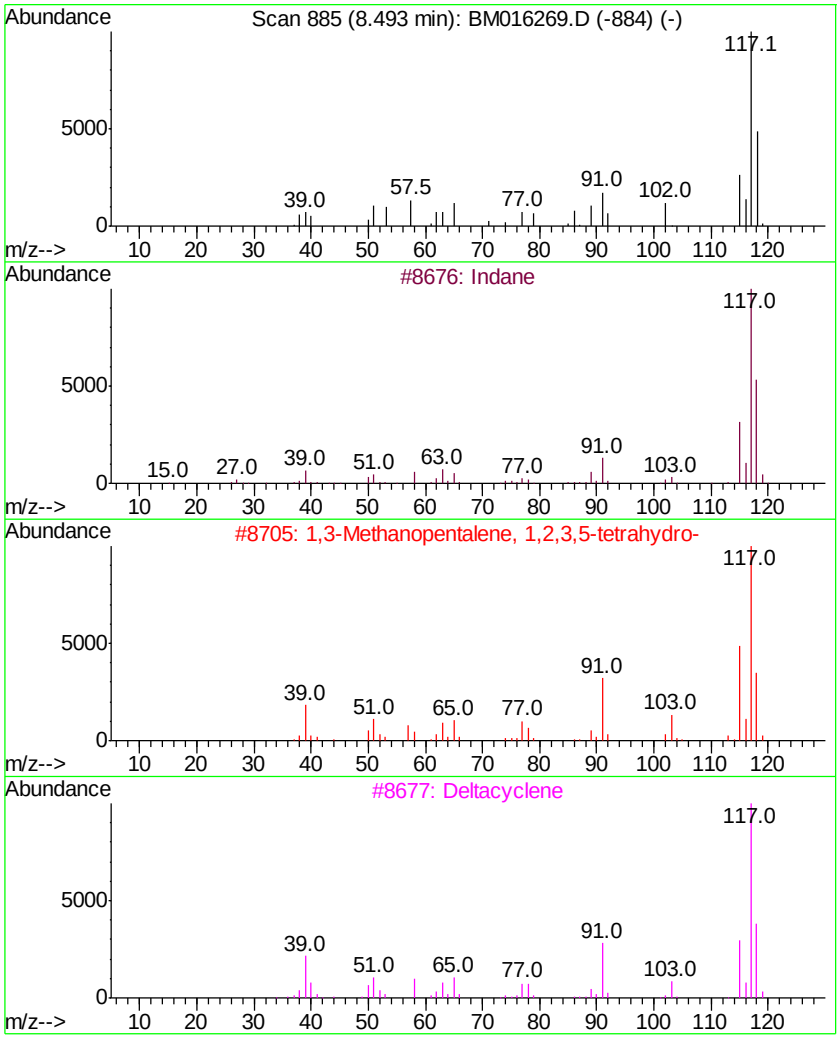
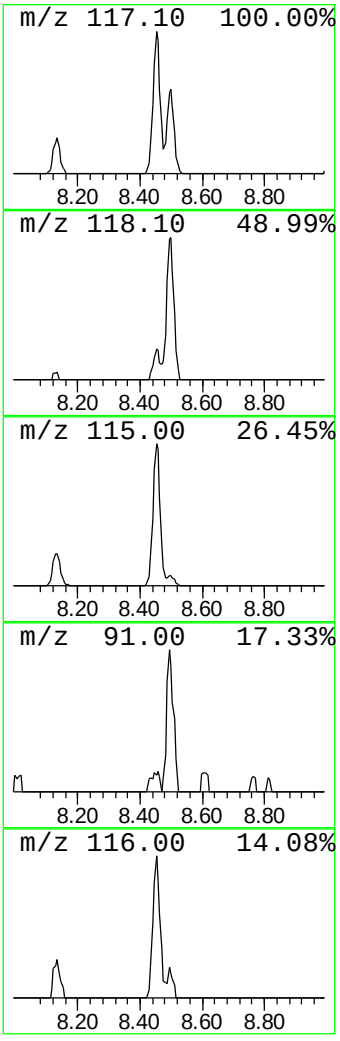
Peak Number 5 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.49	3.76 ng	68269	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	64
2	1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	64
3	Deltacyclene	118	C9H10	007785-10-6	64
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	59





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Sample : J4328-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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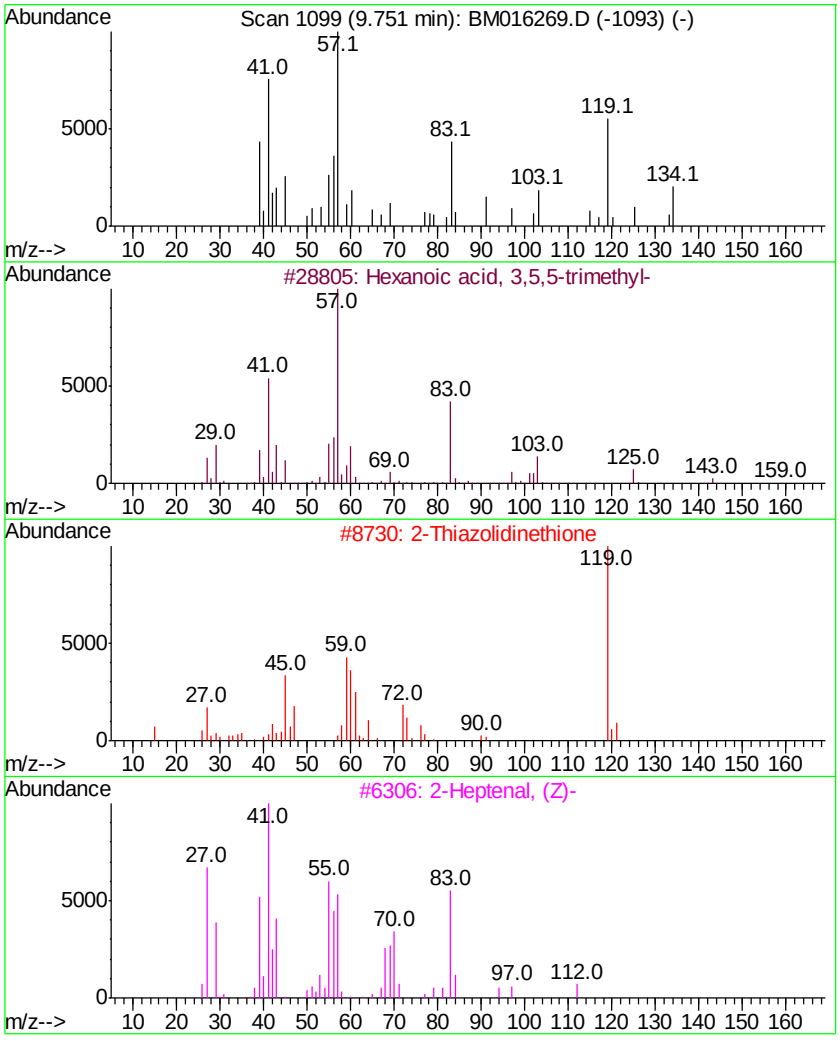
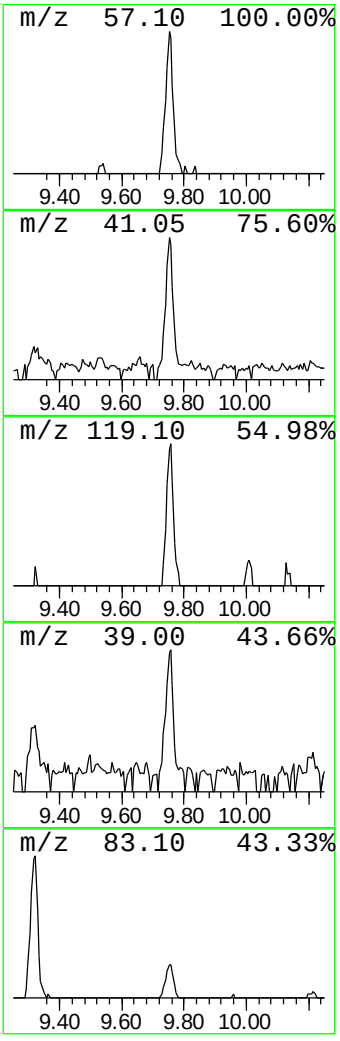
****

Peak Number 6 Hexanoic acid, 3,5,5-trimet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	3.38 ng	65952	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	50
2	2-Thiazolidinethione	119	C3H5NS2	000096-53-7	30
3	2-Heptenal, (Z)-	112	C7H12O	057266-86-1	22
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	18
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	18





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Sample : J4328-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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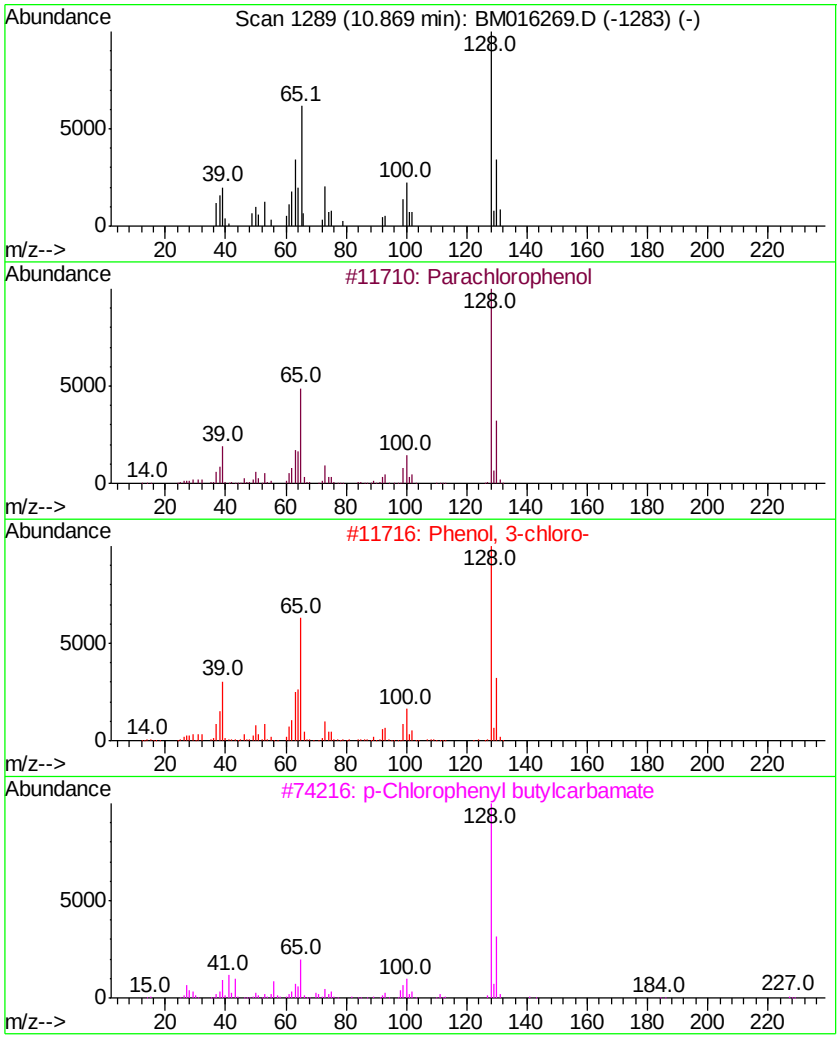
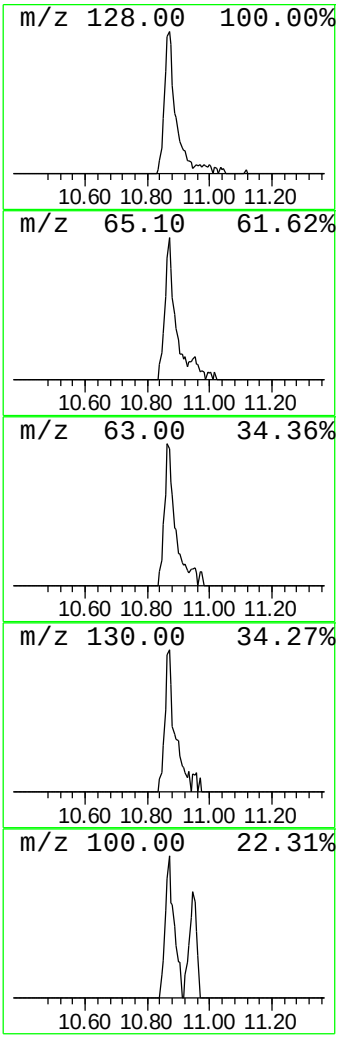
Peak Number 7 Parachlorophenol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	6.02 ng	117585	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Parachlorophenol	128	C6H5ClO	000106-48-9	91
2	Phenol, 3-chloro-	128	C6H5ClO	000108-43-0	90
3	p-Chlorophenyl butylcarbamate	227	C11H14ClNO2	132905-93-2	72
4	p-Chlorophenyl N-(cyanomethyl)ca...	210	C9H7ClN2O2	1000240-68-8	50
5	3-Chloro-6-methylpyridazine	128	C5H5ClN2	001121-79-5	38





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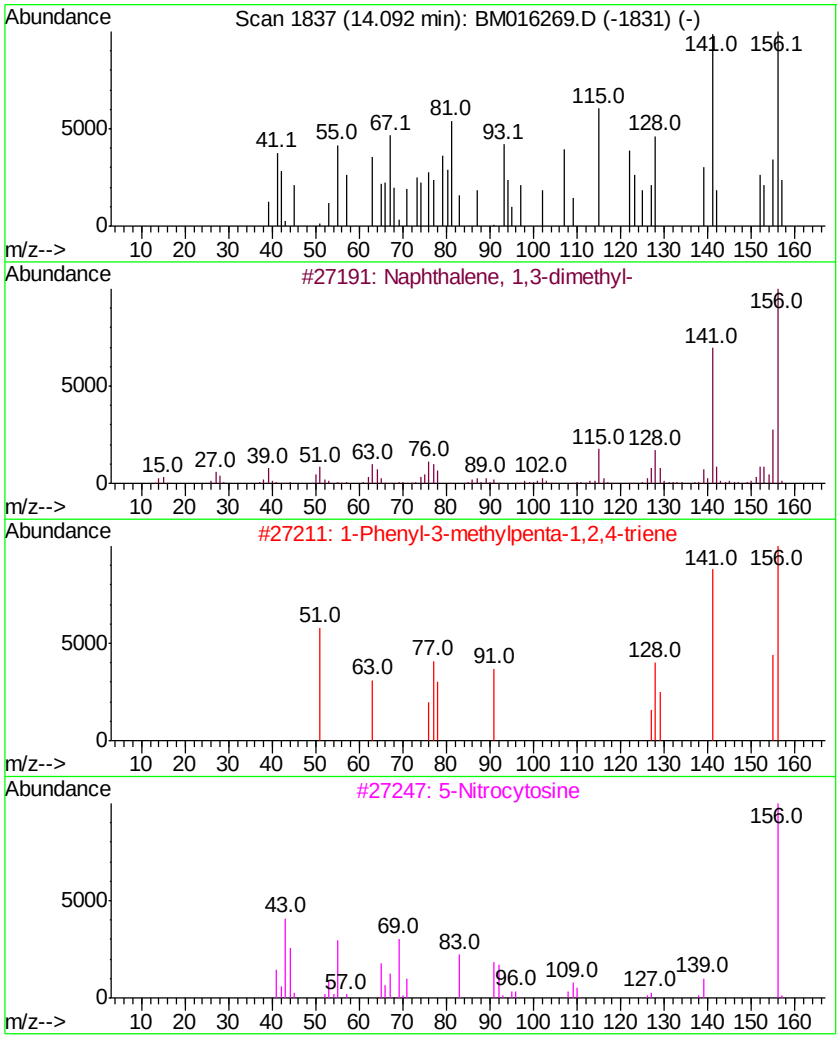
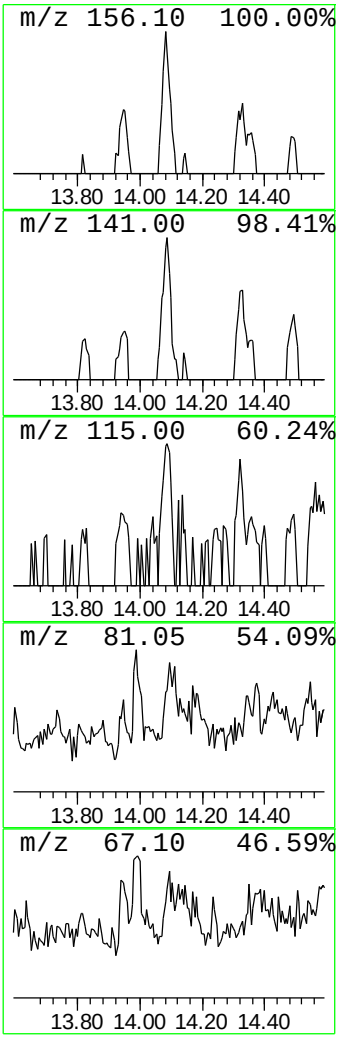
Peak Number 8 Naphthalene, 1,3-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	2.93 ng	66166	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	58
2	1-Phenyl-3-methylpenta-1,2,4-triene	156	C12H12	093247-38-2	12
3	5-Nitrocytosine	156	C4H4N4O3	069099-99-6	10
4	Cyclohexanecarboxamide, 2-oxo-	141	C7H11NO2	022945-27-3	9
5	6-Methyl-2-mercaptopyridine-1-oxide	141	C6H7NOS	051583-70-1	9





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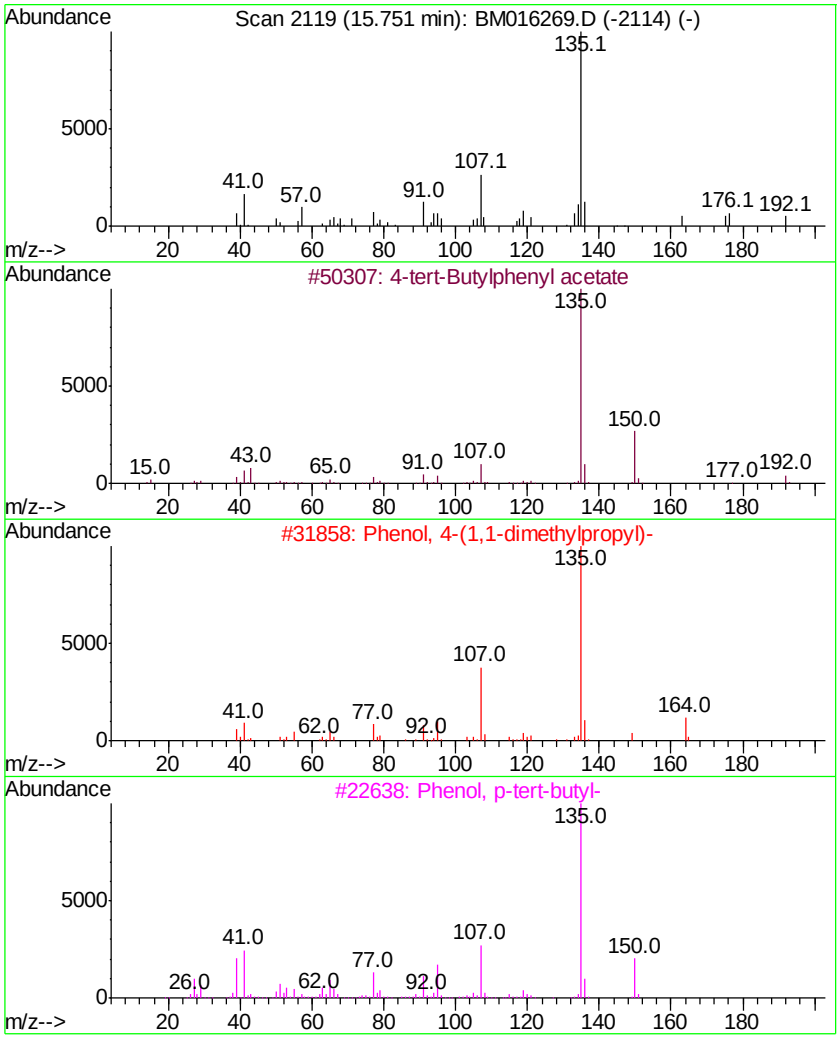
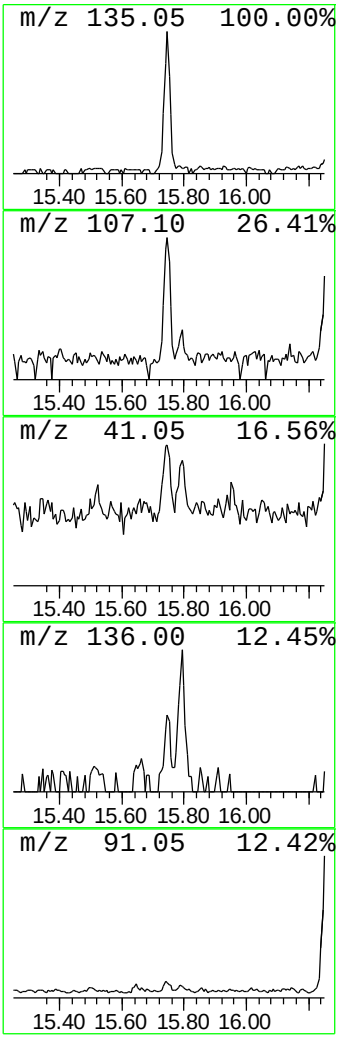
****

Peak Number 10 4-tert-Butylphenyl acetate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	2.06 ng	46363	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	72
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72
4	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	64
5	Phenol, 5-methyl-2-(1-methylethy...	192	C12H16O2	000528-79-0	59





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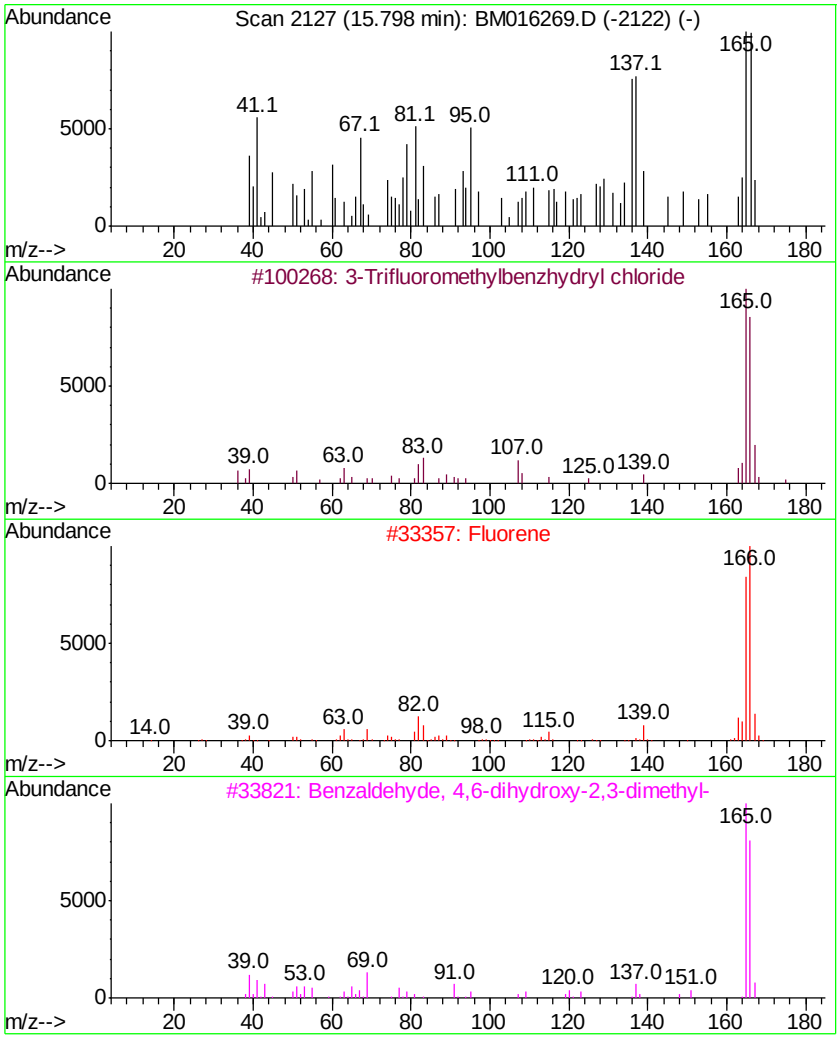
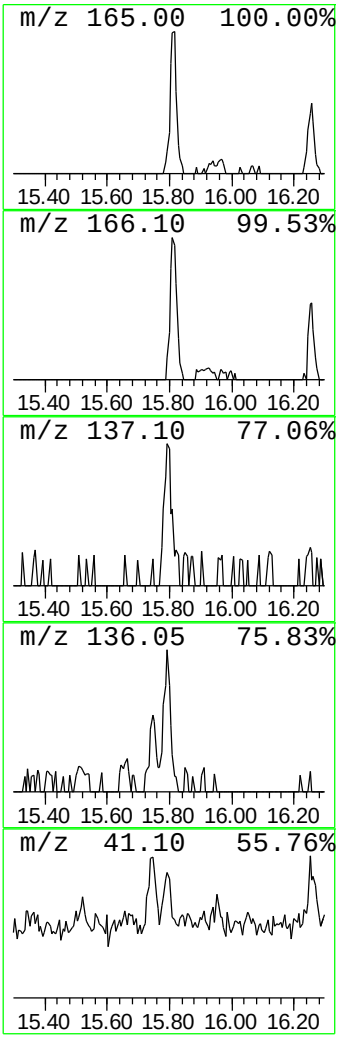
****

Peak Number 11 3-Trifluoromethylbenzhydryl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	3.74 ng	84280	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Trifluoromethylbenzhydryl chlo...	270	C14H10ClF3	067240-79-3	64
2	Fluorene	166	C13H10	000086-73-7	59
3	Benzaldehyde, 4,6-dihydroxy-2,3-...	166	C9H10O3	002990-31-0	53
4	Benzaldehyde, 2-hydroxy-4-methox...	166	C9H10O3	034883-08-4	52
5	Benzaldehyde, 2,4-dihydroxy-3,6-...	166	C9H10O3	034883-14-2	40





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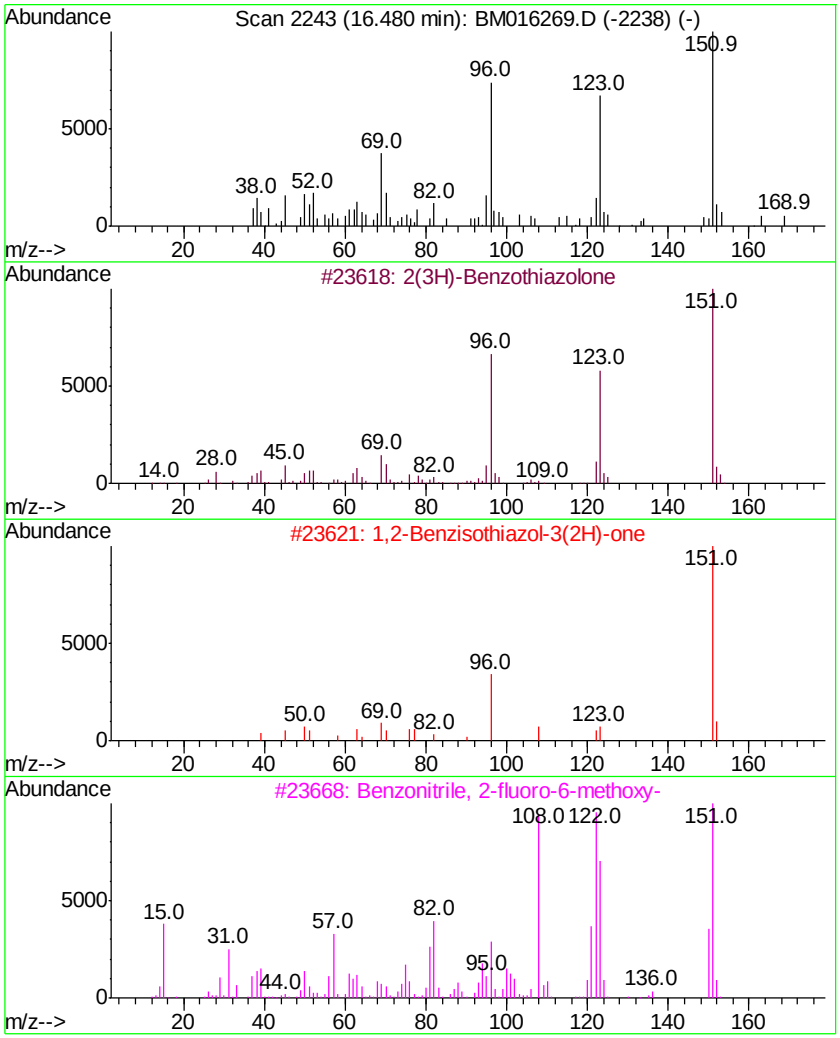
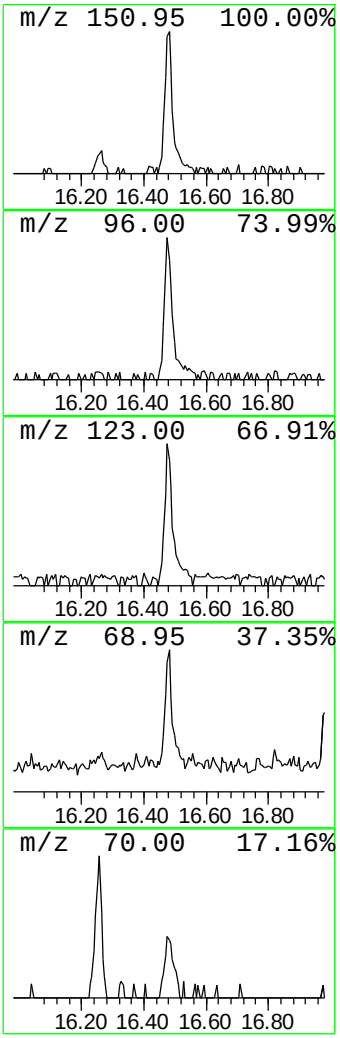
Peak Number 12 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	3.99 ng	99369	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	81
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	64
3	Benzonitrile, 2-fluoro-6-methoxy-	151	C8H6FNO	094088-46-7	52
4	Thieno[3,2-c]pyridin-4(5H)-one	151	C7H5NOS	027685-92-3	52
5	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016269.D
Acq On : 09 Aug 2018 04:39
Operator : SJ/JU
Sample : J4328-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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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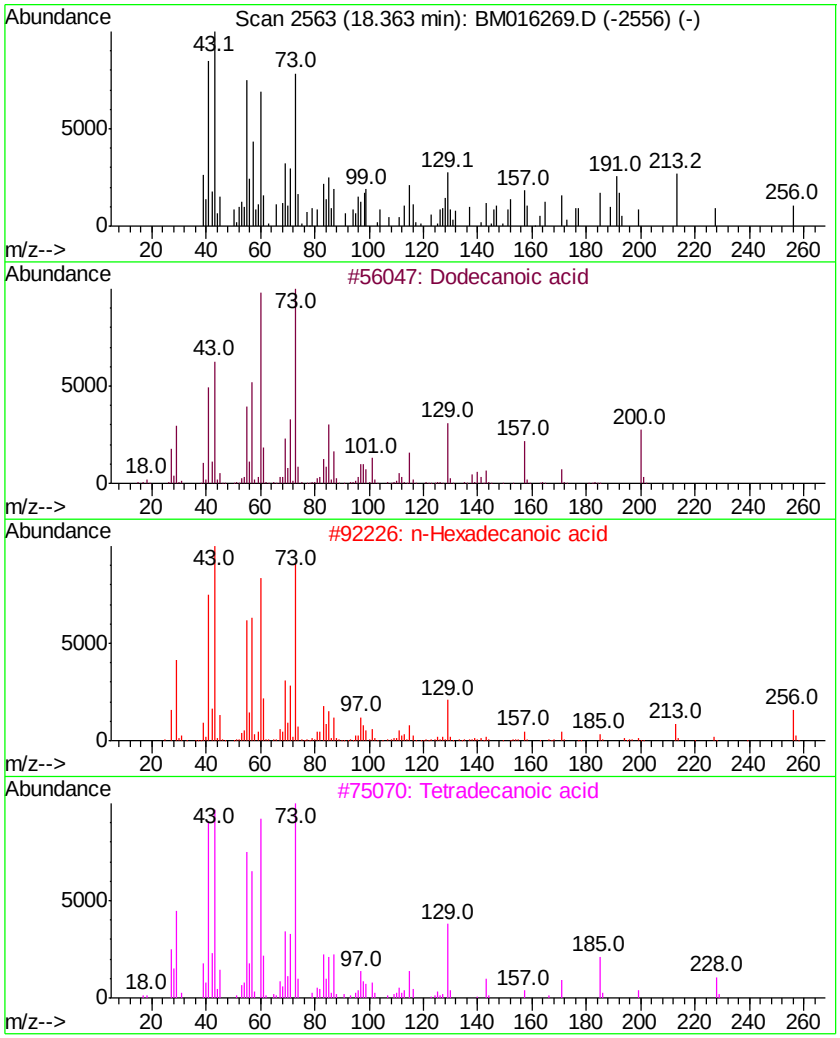
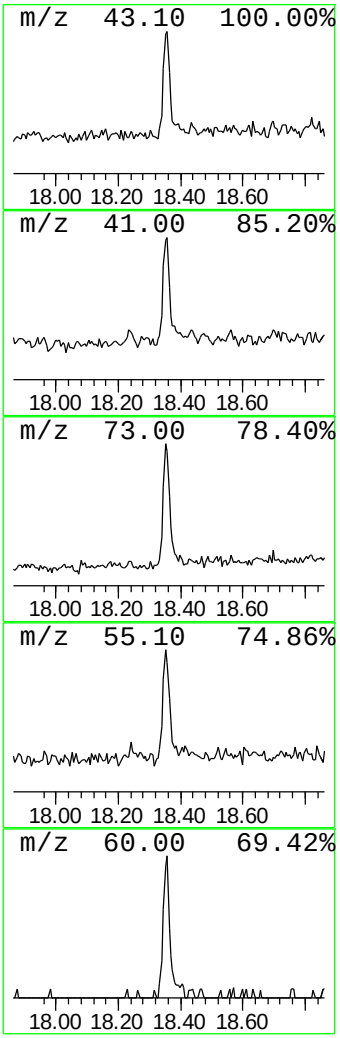
Peak Number 13 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	5.01 ng	124933	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-24

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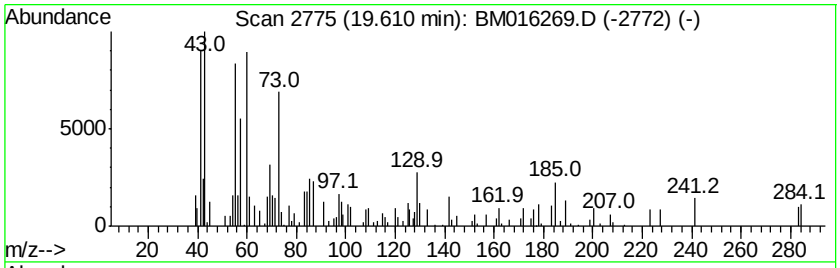
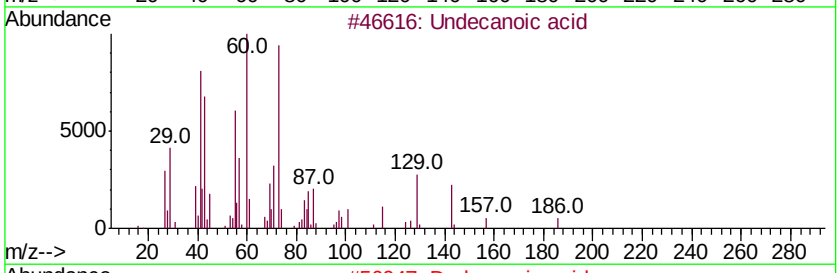
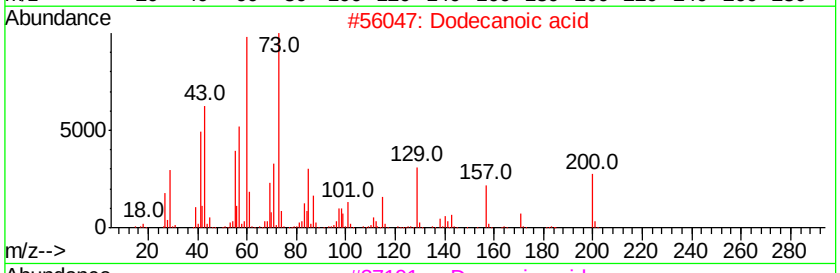
Peak Number 14 Undecanoic acid Concentration Rank 14

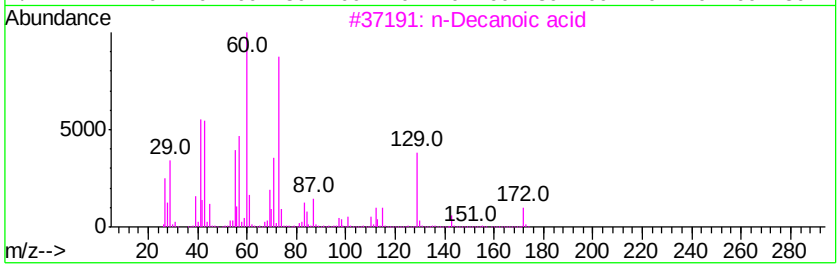
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	2.13 ng	61022	Chrysene-d12	21.63

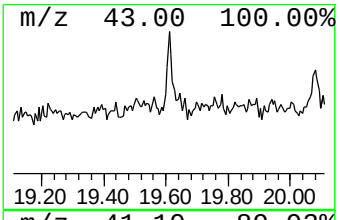
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	52
2	Dodecanoic acid	200	C12H24O2	000143-07-7	49
3	n-Decanoic acid	172	C10H20O2	000334-48-5	46
4	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	37
5	Octanoic Acid	144	C8H16O2	000124-07-2	35

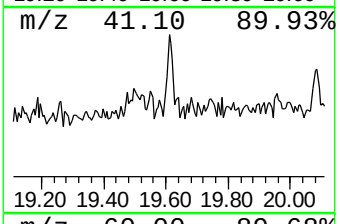


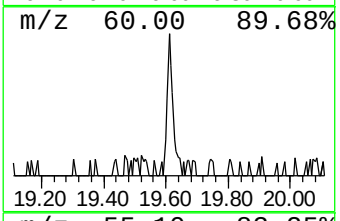


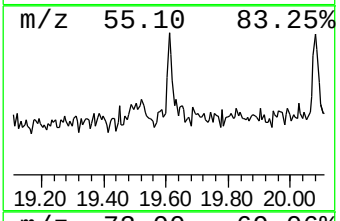


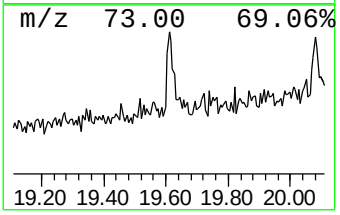












Library Search Compound Report

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-24

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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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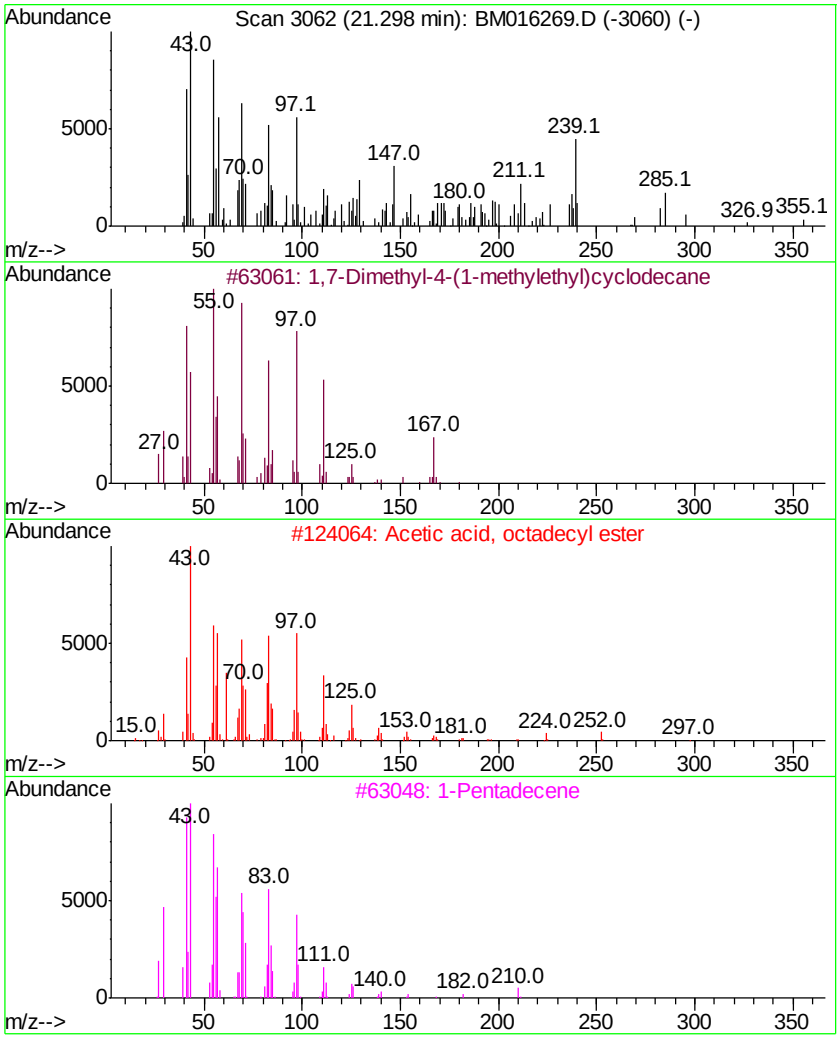
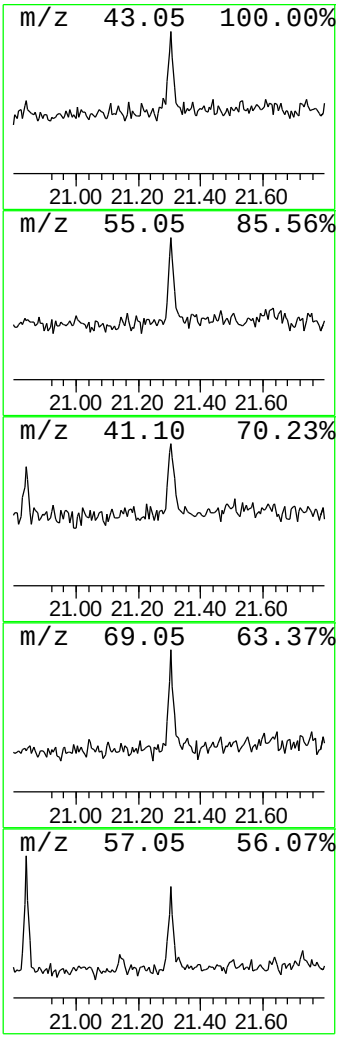
Peak Number 15 unknown Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	2.78 ng	79630	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	45
2	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	43
3	1-Pentadecene	210	C15H30	013360-61-7	41
4	3-Octadecene, (E)-	252	C18H36	007206-19-1	38
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080818\
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	4.0	ng	71763	1	8.13	363109	20.0
unknown7.66	7.66	78.0	ng	1415660	1	8.13	363109	20.0
Indane	8.49	3.8	ng	68269	1	8.13	363109	20.0
Hexanoic acid, 3,...	9.75	3.4	ng	65952	2	10.95	390817	20.0
Parachlorophenol	10.87	6.0	ng	117585	2	10.95	390817	20.0
Naphthalene, 1,3-...	14.09	2.9	ng	66166	3	14.77	450911	20.0
4-tert-Butylpheny...	15.75	2.1	ng	46363	3	14.77	450911	20.0
3-Trifluoromethyl...	15.80	3.7	ng	84280	3	14.77	450911	20.0
2(3H)-Benzothiazo...	16.48	4.0	ng	99369	4	17.50	498376	20.0
Dodecanoic acid	18.36	5.0	ng	124933	4	17.50	498376	20.0
Undecanoic acid	19.61	2.1	ng	61022	5	21.63	571914	20.0
unknown	21.30	2.8	ng	79630	5	21.63	571914	20.0