LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042421\
Data File : BM029647.D
Acq On : 24 Apr 2021 20:56
Operator : CG/JU
Sample : M2118-03 20X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 20071

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-BM042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029647.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.622	791	805	813	rBV	349944	563957	9.37%	3.441%
2	10.404	1271	1278	1287	rBV	420793	707689	11.75%	4.319%
3	14.268	1930	1935	1948	rVB	643462	970766	16.12%	5.924%
4	16.415	2296	2300	2305	rVB	147181	192278	3.19%	1.173%
5	16.480	2308	2311	2316	rVB	59964	79285	1.32%	0.484%
6	17.015	2397	2402	2409	rBV	754767	1072766	17.82%	6.546%
7	17.092	2412	2415	2422	rVB	116591	157661	2.62%	0.962%
8	17.809	2533	2537	2541	rVB3	69756	114220	1.90%	0.697%
9	18.398	2634	2637	2640	rBV	108660	138095	2.29%	0.843%
10	18.774	2697	2701	2707	rVB	182169	237192	3.94%	1.447%
11	19.321	2791	2794	2801	rVB	143311	164642	2.73%	1.005%
12	20.421	2978	2981	2985	rVB2	257991	298444	4.96%	1.821%
13	20.592	3007	3010	3014	rBV	184258	190962	3.17%	1.165%
14	21.197	3109	3113	3119	rBV	1077463	1294649	21.50%	7.900%
15	21.991	3245	3248	3252	rBV	419673	494580	8.21%	3.018%
16	24.427	3657	3662	3672	rVB	1472642	3688529	61.25%	22.508%
17	25.074	3767	3772	3783	rVB	2572041	6021650	100.00%	36.746%

Sum of corrected areas: 16387365

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BNA_M
ClientSampleId :
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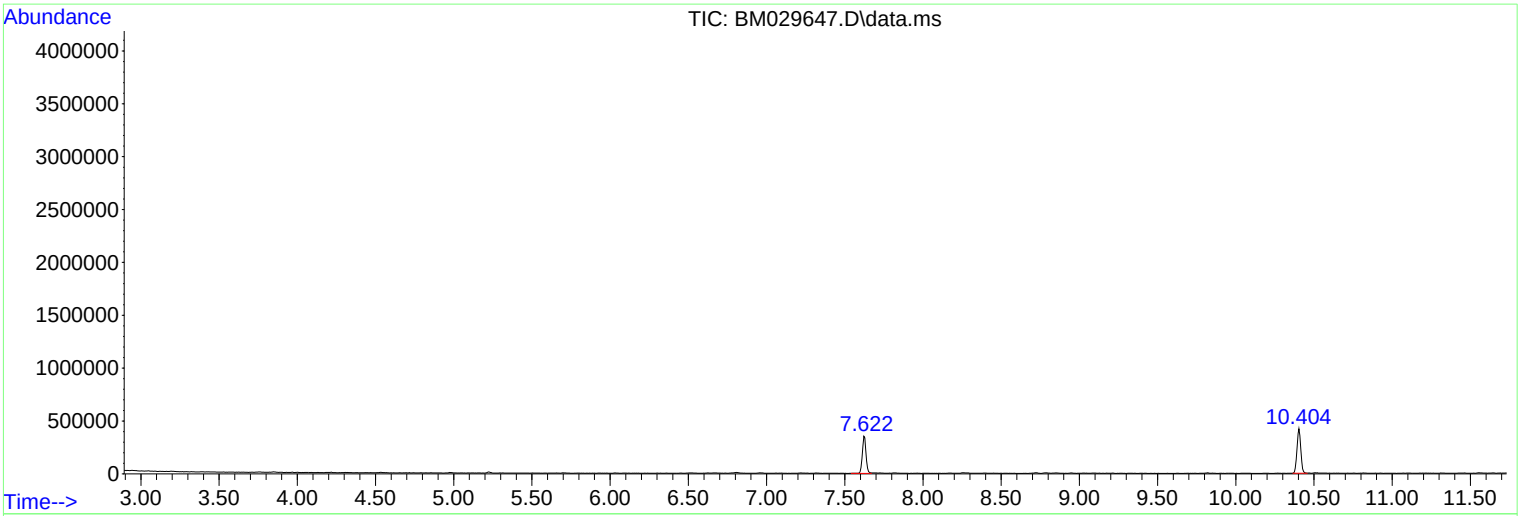
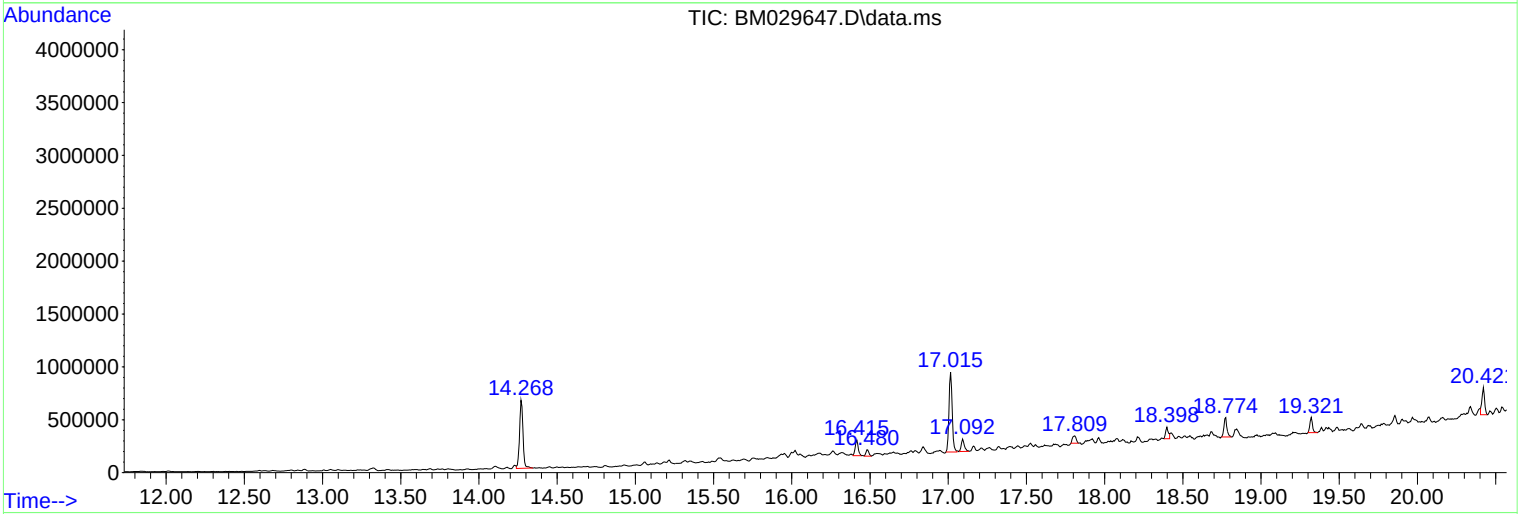
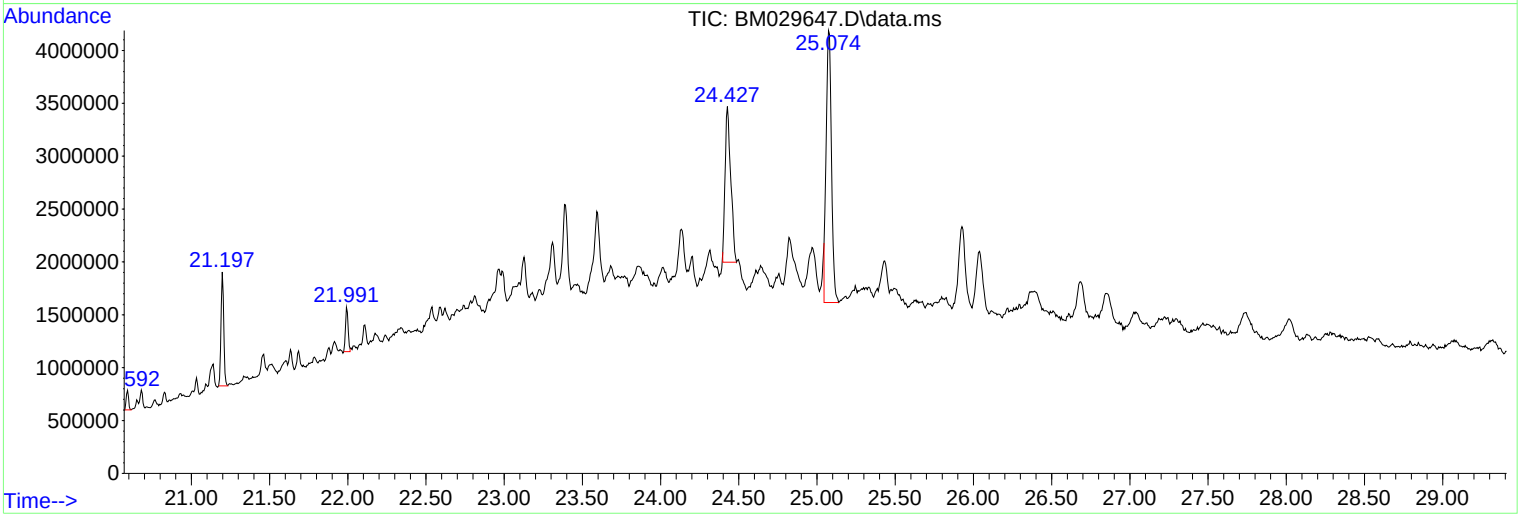
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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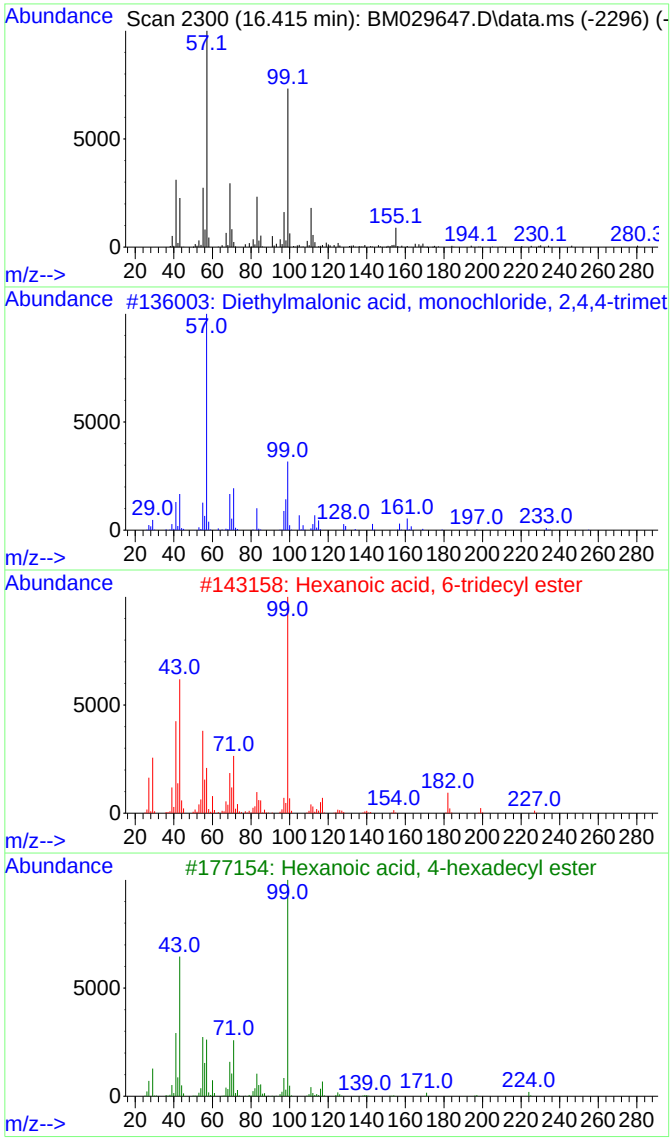
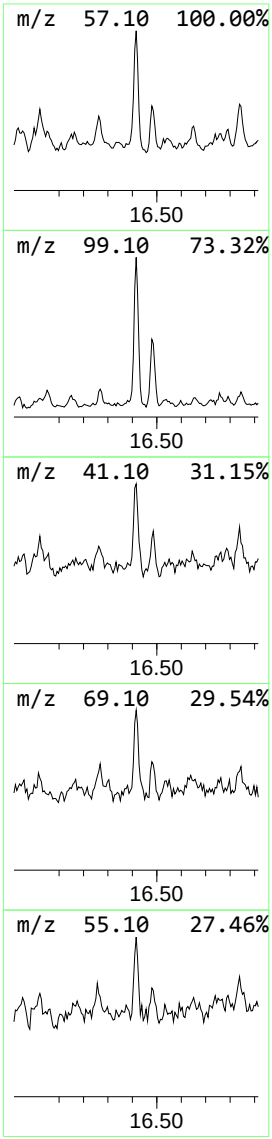
****
Peak Number 1 Diethylmalonic acid, monoch... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.415	3.58 ng	192278	Phenanthrene-d10	17.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylmalonic acid, monochlorid...	290	C15H27ClO3	1000369-49-2	56
2	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	47
3	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	47
4	Didodecyl phosphate	434	C24H51O4P	007057-92-3	47
5	cis-4-Hydroxy-3-methylundecanoic...	198	C12H22O2	148806-09-1	43





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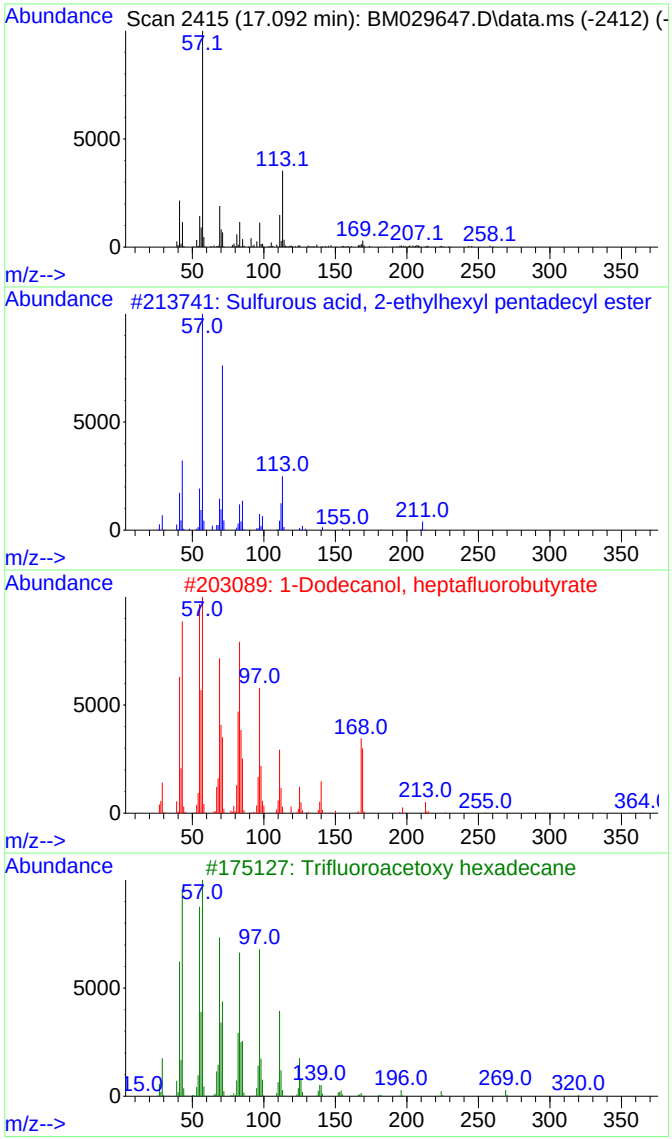
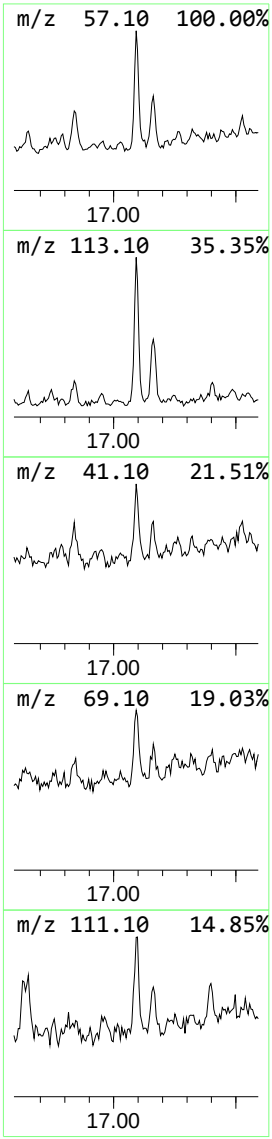
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Sulfurous acid, 2-ethylhexy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.092	2.94 ng	157661	Phenanthrene-d10	17.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl pen...	404	C23H48O3S	1000309-19-8	50
2	1-Dodecanol, heptafluorobutyrate	382	C16H25F7O2	006222-08-8	38
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	38
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	38
5	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	38





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Instrument : BNA_M
ClientSampleId : 20071

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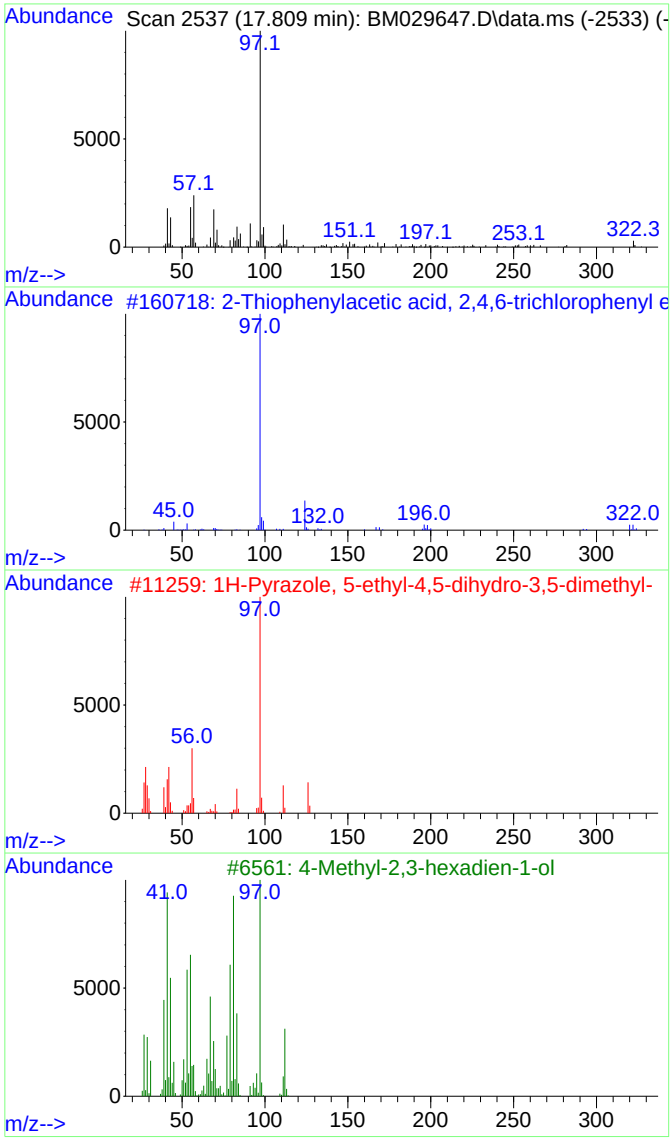
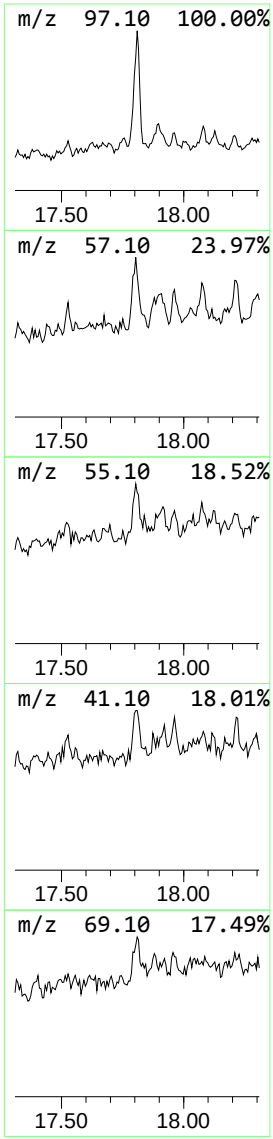
****
Peak Number 3 2-Thiophenylacetic acid, 2,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.809	2.13 ng	114220	Phenanthrene-d10	17.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenylacetic acid, 2,4,6-t...	320	C12H7Cl3O2S	1000325-72-0	64
2	1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	59
3	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	53
4	Heptane, 1,7-dibromo-	256	C7H14Br2	004549-31-9	53
5	Thiophene, 2-heptyl-	182	C11H18S	018794-78-0	50





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Instrument : BNA_M
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TIC Library : C:\DATABASE\NIST11.L
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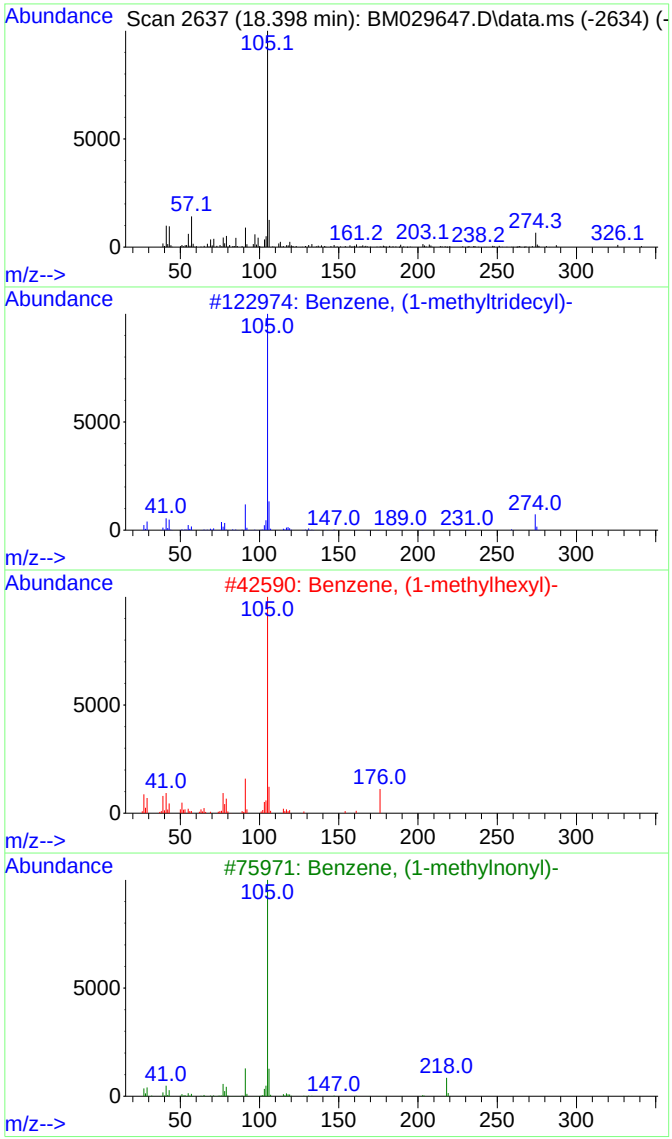
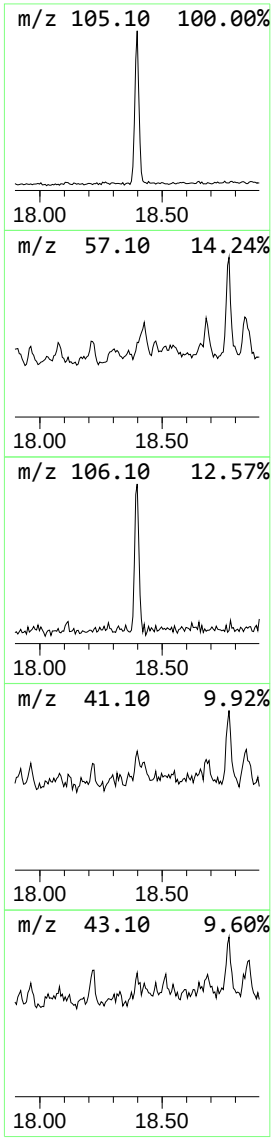
****
Peak Number 4 Benzene, (1-methyltridecyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.398	2.57 ng	138095	Phenanthrene-d10	17.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	72
2	Benzene, (1-methylhexyl)-	176	C13H20	002132-84-5	58
3	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	53
4	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	53
5	Benzene, (1-methylheptadecyl)-	330	C24H42	006583-67-1	50





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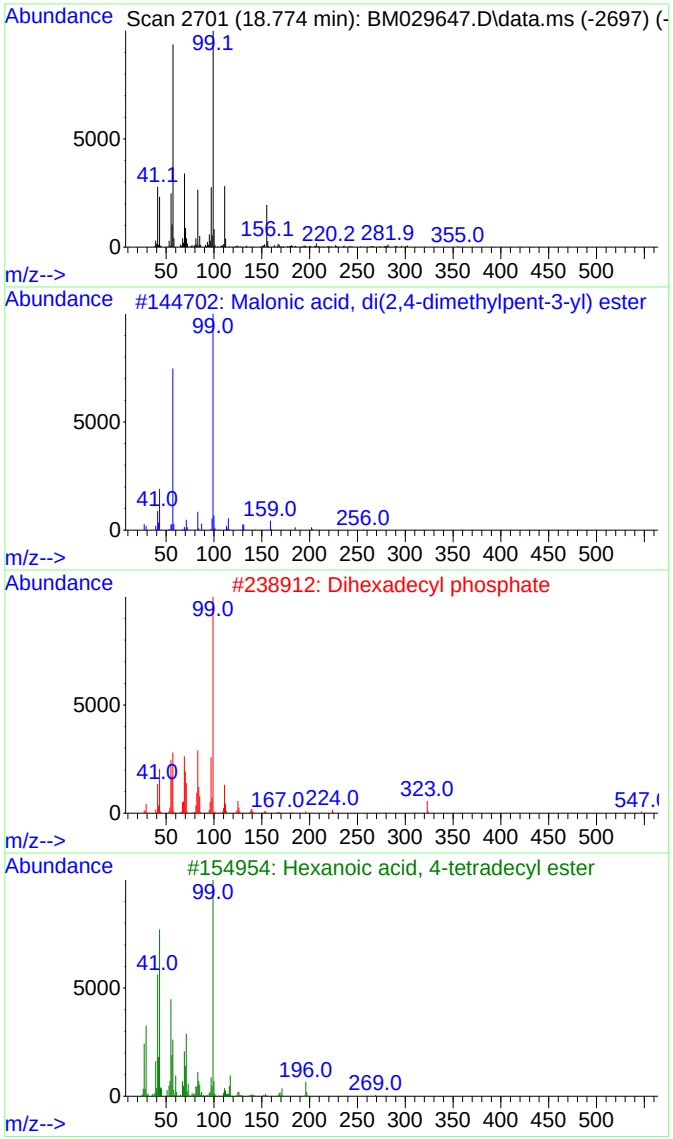
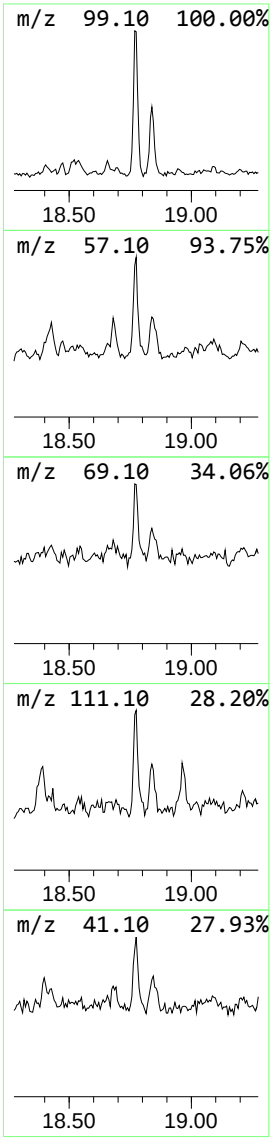
****

Peak Number 5 unknown18.774 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.774	4.42 ng	237192	Phenanthrene-d10	17.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malonic acid, di(2,4-dimethylpen...	300	C17H32O4	1000349-02-5	43
2	Dihexadecyl phosphate	546	C32H67O4P	002197-63-9	40
3	Hexanoic acid, 4-tetradecyl ester	312	C20H40O2	1000279-29-8	38
4	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	38
5	Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	38





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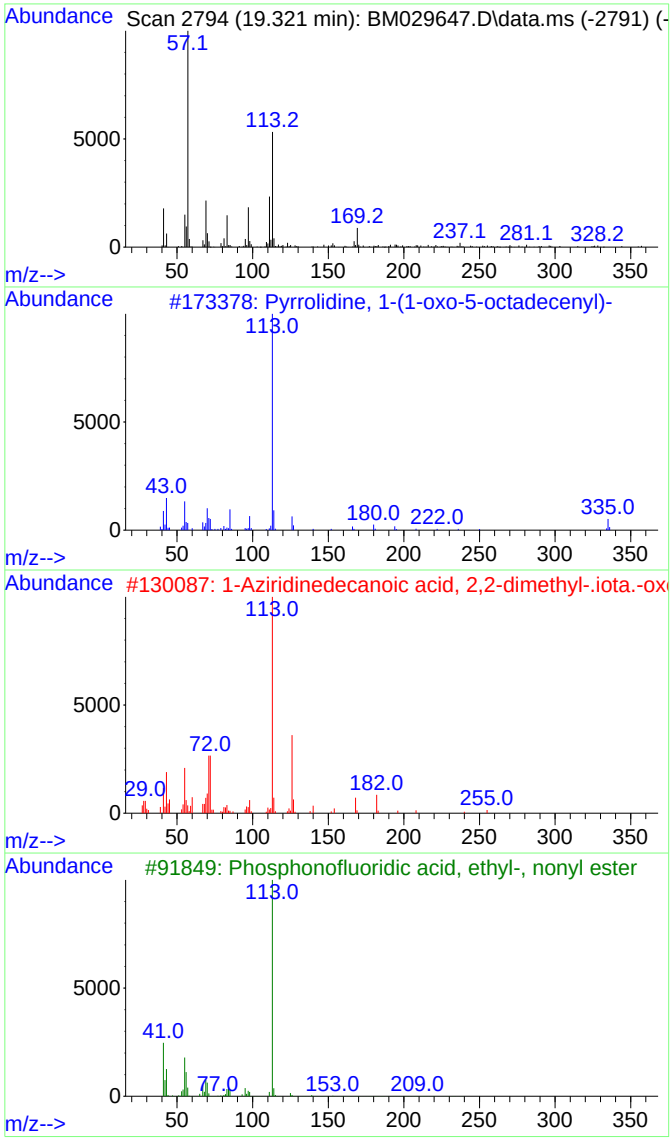
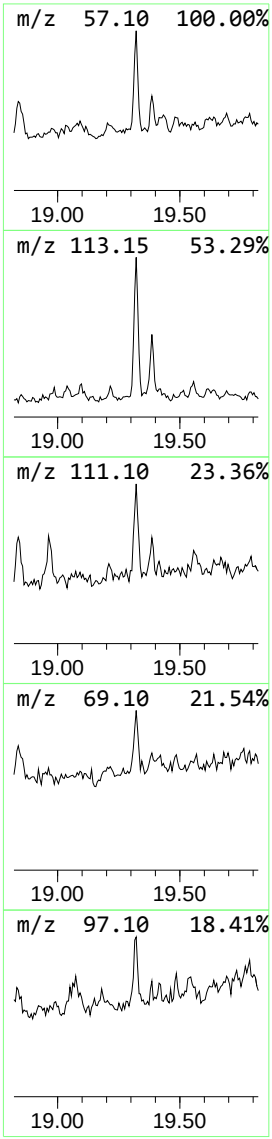
****

Peak Number 6 unknown19.321 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.321	2.54 ng	164642	Chrysene-d12	21.197

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolidine, 1-(1-oxo-5-octadece...	335	C22H41NO	056599-67-8	35
2	1-Aziridinedecanoic acid, 2,2-di...	283	C16H29NO3	056817-99-3	27
3	Phosphonofluoridic acid, ethyl-,...	238	C11H24FO2P	171741-07-4	25
4	Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	25
5	2,6-Piperidinedione, 1-(5-hydrox...	199	C10H17NO3	1000115-16-1	25





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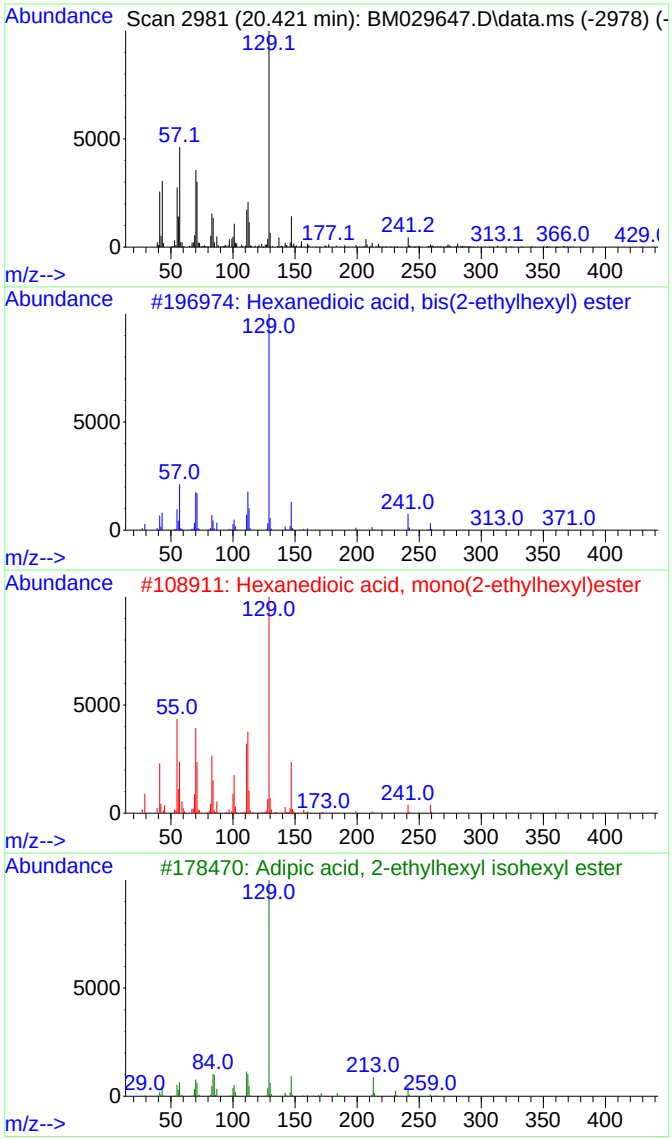
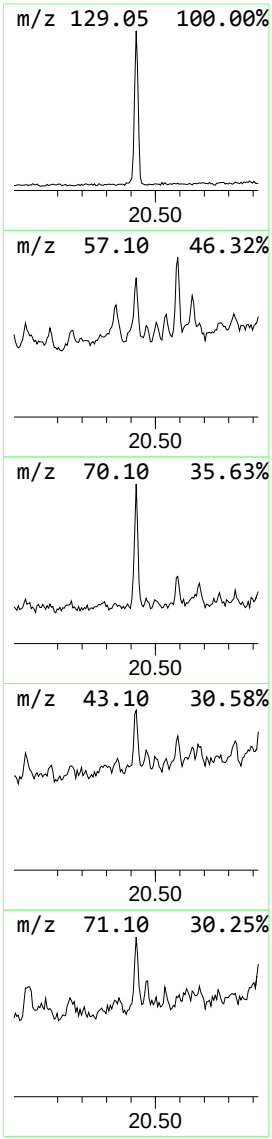
****
Peak Number 7 Hexanedioic acid, bis(2-eth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.421	4.61 ng	298444	Chrysene-d12	21.197

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58
3	Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	53
4	Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	53
5	Adipic acid, isohexyl octyl ester	342	C20H38O4	1000324-47-0	50





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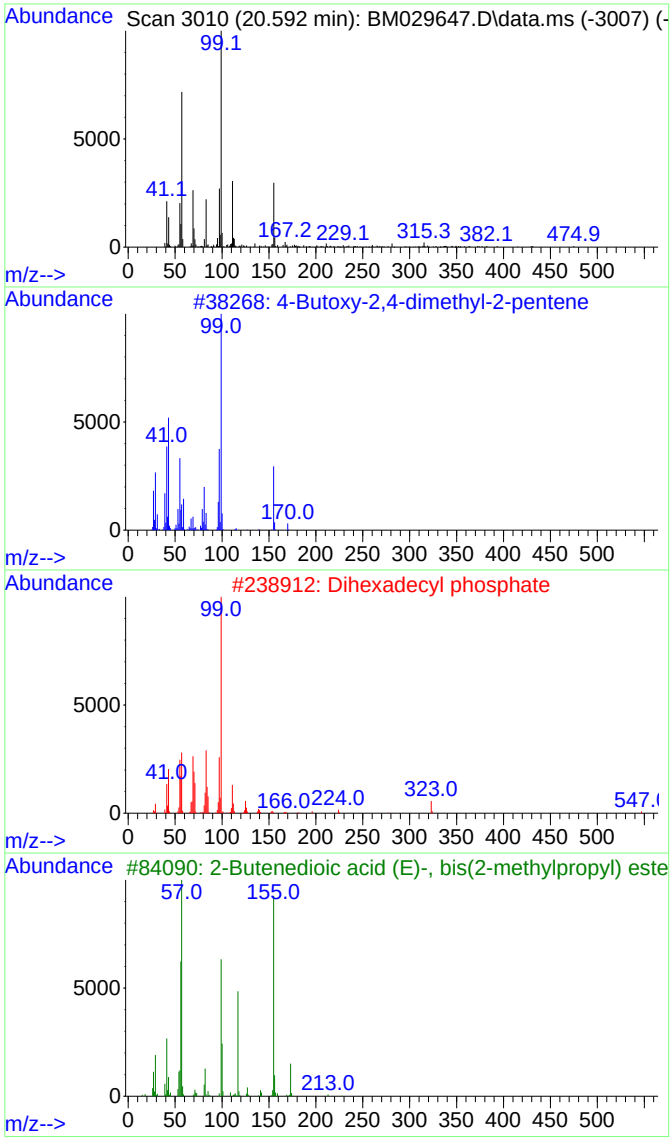
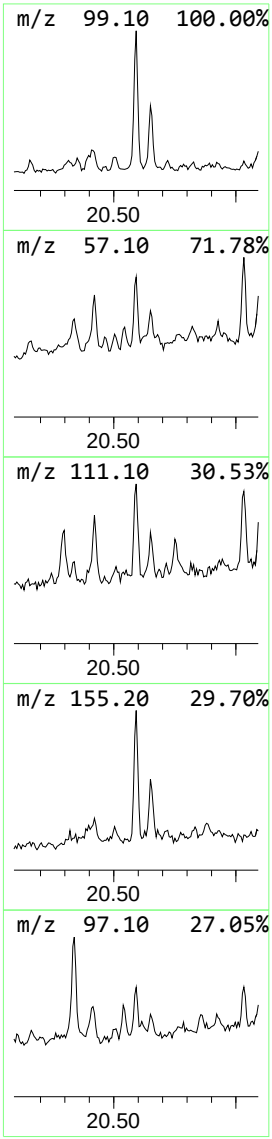
****

Peak Number 8 4-Butoxy-2,4-dimethyl-2-pen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.592	2.95 ng	190962	Chrysene-d12	21.197

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	53
2	Dihexadecyl phosphate	546	C32H67O4P	002197-63-9	45
3	2-Butenedioic acid (E)-, bis(2-m...	228	C12H20O4	007283-69-4	38
4	N-Phenyl-N'-(2-piperazin-1-yl-et...	276	C14H20N4O2	332404-00-9	38
5	Spiro[1,3-dioxolane-2,2'-[6,7]di...	182	C9H14N2O2	1000142-34-9	37





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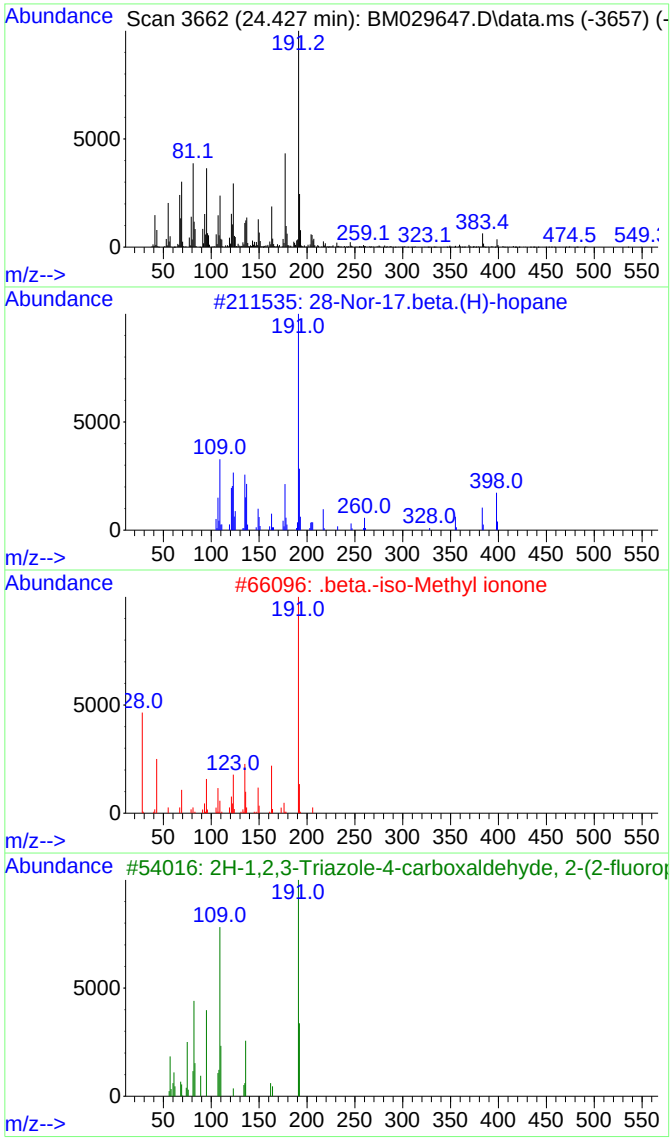
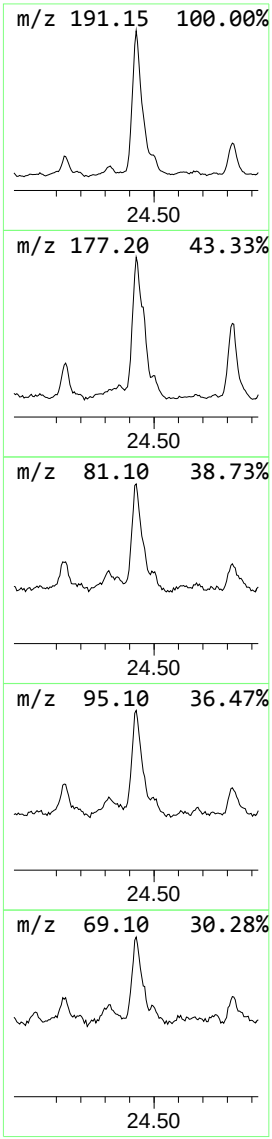
****

Peak Number 9 28-Nor-17.beta.(H)-hopane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.427	20.00 ng	3688530	Perylene-d12	23.391

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	58
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
3	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	43
4	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	30
5	2-Amino-4-methyl-6-(2-thienyl)py...	191	C9H9N3S	026963-43-9	27





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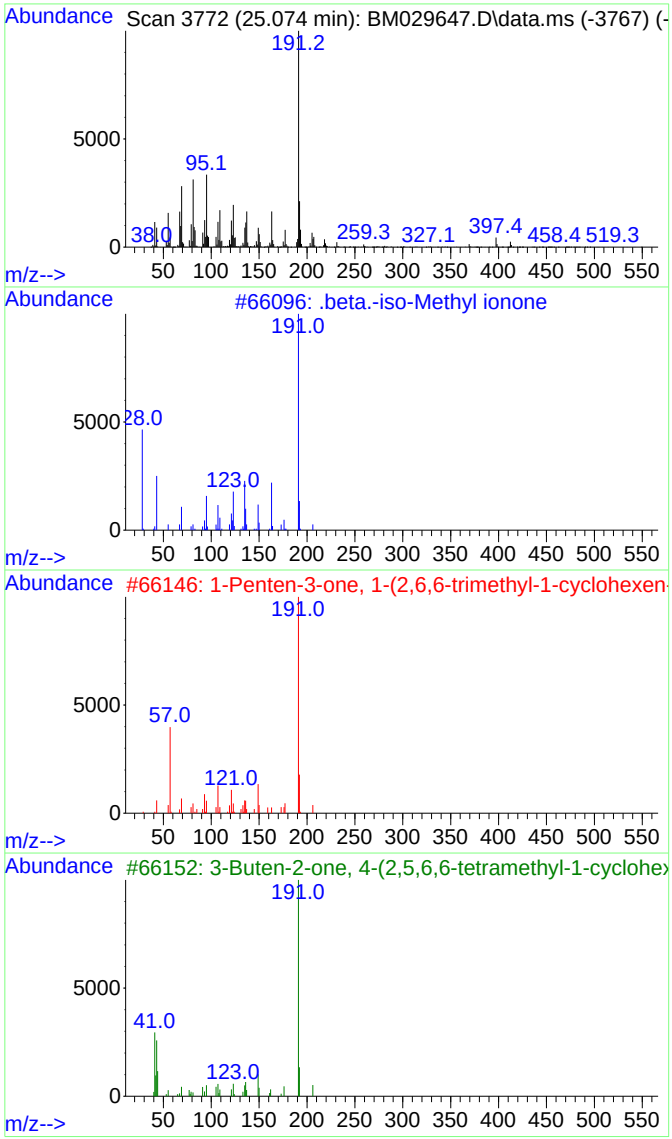
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

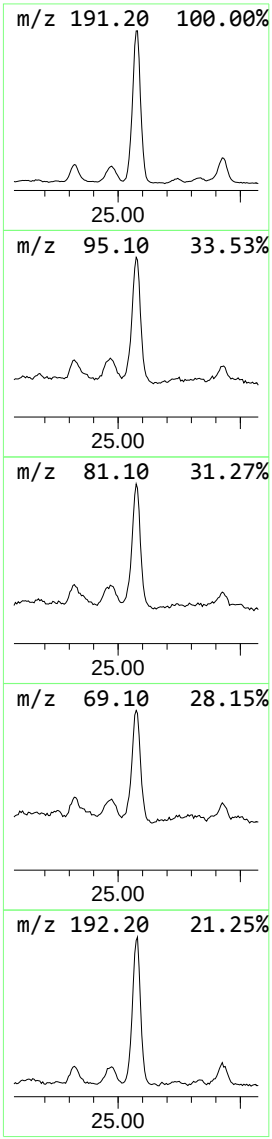
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 .beta.-iso-Methyl ionone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.074	32.65 ng	6021650	Perylene-d12	23.391

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	81
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	70
3	3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	47
4	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	47
5	4-Fluoro-3-trifluoromethylbenzoi...	390	C21H30F4O2	1000338-67-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042421\
Data File : BM029647.D
Acq On : 24 Apr 2021 20:56
Operator : CG/JU
Sample : M2118-03 20X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 20071

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
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
Diethylmalonic ...	16.415	3.6	ng	192278	4	17.015	1072770	20.0
Sulfurous acid,...	17.092	2.9	ng	157661	4	17.015	1072770	20.0
2-Thiophenylace...	17.809	2.1	ng	114220	4	17.015	1072770	20.0
Benzene, (1-met...	18.398	2.6	ng	138095	4	17.015	1072770	20.0
unknown18.774	18.774	4.4	ng	237192	4	17.015	1072770	20.0
unknown19.321	19.321	2.5	ng	164642	5	21.197	1294650	20.0
Hexanedioic aci...	20.421	4.6	ng	298444	5	21.197	1294650	20.0
4-Butoxy-2,4-di...	20.592	3.0	ng	190962	5	21.197	1294650	20.0
28-Nor-17.beta....	24.427	20.0	ng	3688530	6	23.391	3688530	20.0
.beta.-iso-Meth...	25.074	32.6	ng	6021650	6	23.391	3688530	20.0