LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
Data File : BM035398.D
Acq On : 03 Jun 2022 16:56
Operator : CG/JU
Sample : N3143-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20220425-AMENDED-COMP-E

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-BM060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035398.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	314	321	343	rBV	4591370	6674200	78.85%	14.547%
2	5.440	394	400	407	rBV	196388	311065	3.68%	0.678%
3	7.034	662	671	686	rVB	962899	1628621	19.24%	3.550%
4	7.845	802	809	817	rBV	535225	872950	10.31%	1.903%
5	9.010	1000	1007	1021	rBV	1638222	2755180	32.55%	6.005%
6	9.363	1057	1067	1076	rBV	1207701	2088413	24.67%	4.552%
7	10.645	1272	1285	1291	rBV	691271	1186957	14.02%	2.587%
8	13.116	1697	1705	1718	rBV	4497494	6787213	80.19%	14.794%
9	13.233	1719	1725	1729	rBV	99783	167859	1.98%	0.366%
10	13.516	1767	1773	1785	rVB	99295	192162	2.27%	0.419%
11	14.392	1917	1922	1929	rVV	140841	274483	3.24%	0.598%
12	14.486	1930	1938	1945	rVV	1086384	1715007	20.26%	3.738%
13	14.551	1947	1949	1958	rVB3	40195	91103	1.08%	0.199%
14	15.498	2106	2110	2114	rBV	112550	164215	1.94%	0.358%
15	15.980	2188	2192	2198	rBV	231146	360966	4.26%	0.787%
16	16.198	2225	2229	2233	rBV	299797	455191	5.38%	0.992%
17	16.327	2247	2251	2256	rBV	69893	115089	1.36%	0.251%
18	16.645	2301	2305	2311	rVB4	63773	124219	1.47%	0.271%
19	16.998	2359	2365	2371	rBV	453377	749639	8.86%	1.634%
20	17.233	2400	2405	2410	rBV	1288792	1858332	21.96%	4.050%
21	17.274	2410	2412	2419	rVB	308830	409558	4.84%	0.893%
22	17.368	2424	2428	2433	rVB	112091	169605	2.00%	0.370%
23	18.139	2556	2559	2566	rBV2	202624	295888	3.50%	0.645%
24	19.292	2751	2755	2762	rBV	628616	884335	10.45%	1.928%
25	19.415	2774	2776	2785	rVB3	85048	138900	1.64%	0.303%
26	19.656	2813	2817	2827	rVB	579469	872665	10.31%	1.902%
27	19.862	2847	2852	2857	rBV	6742754	8464080	100.00%	18.449%
28	20.315	2926	2929	2933	rVB	168481	203974	2.41%	0.445%
29	21.133	3065	3068	3075	rVB3	330505	470406	5.56%	1.025%
30	21.421	3111	3117	3121	rBV2	1768364	2693714	31.83%	5.871%
31	23.062	3393	3396	3401	rBV2	317663	529303	6.25%	1.154%
32	23.780	3513	3518	3525	rVB2	1158044	2174210	25.69%	4.739%

Sum of corrected areas: 45879502

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ClientSampleId :
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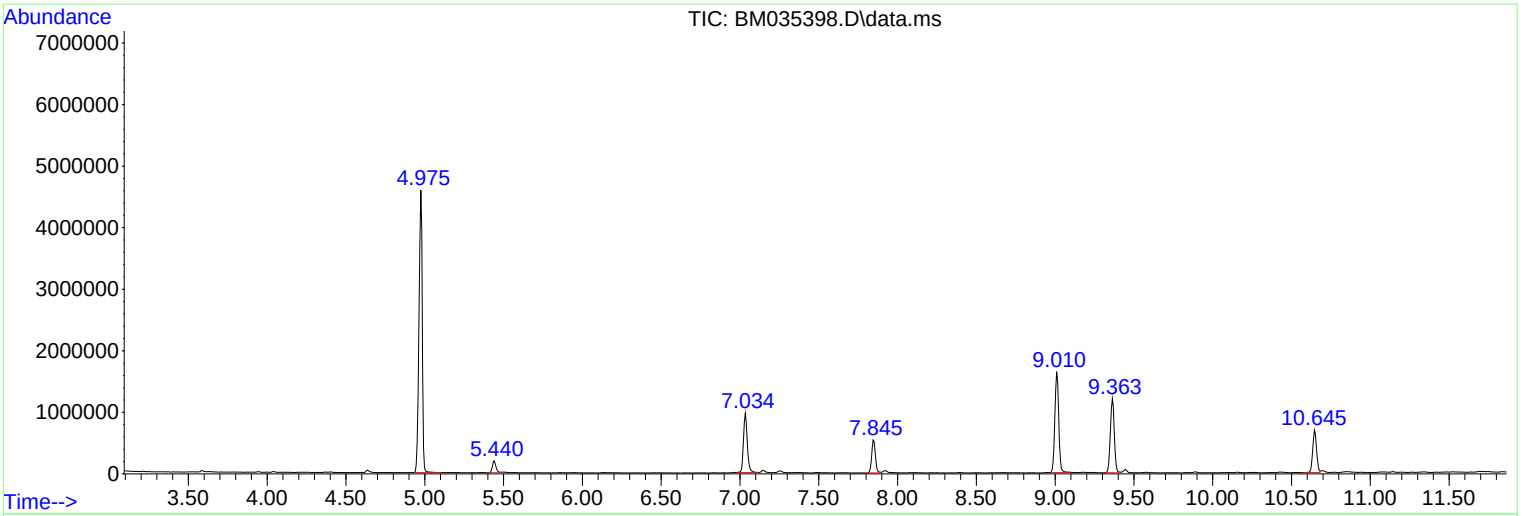
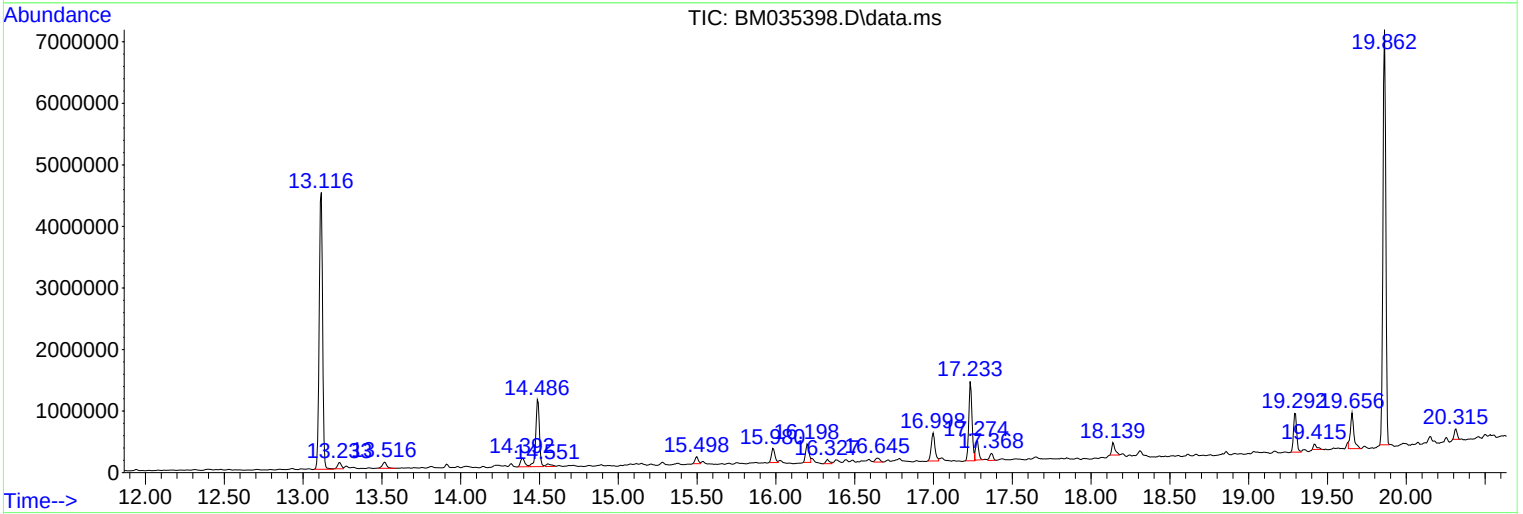
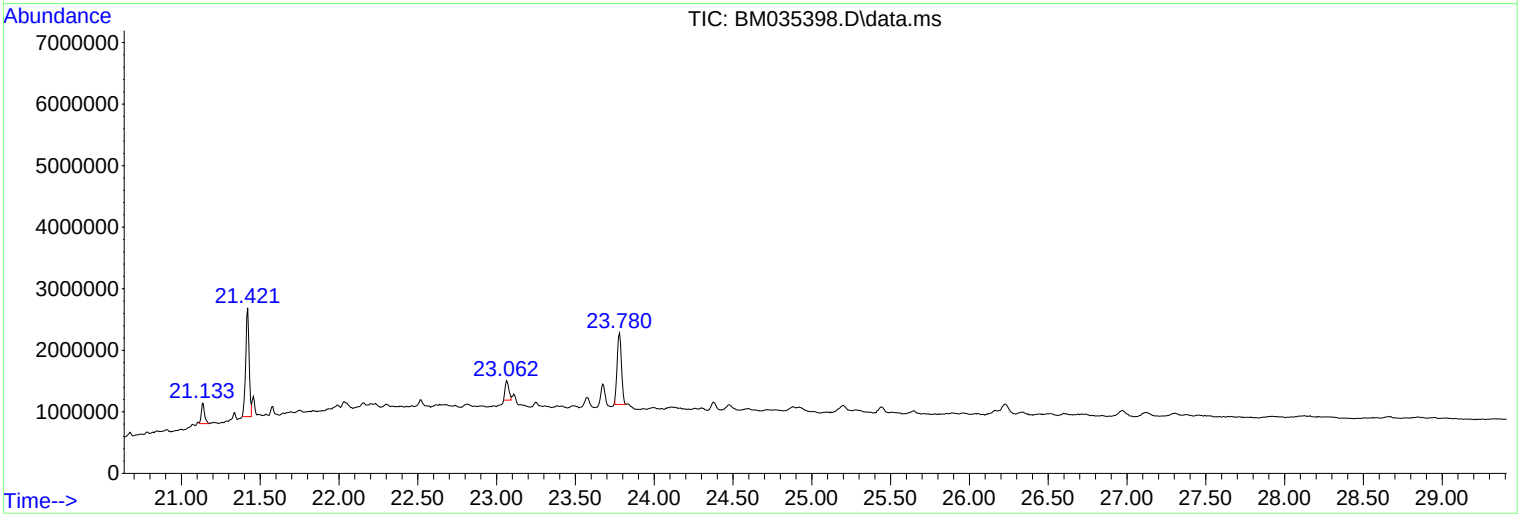
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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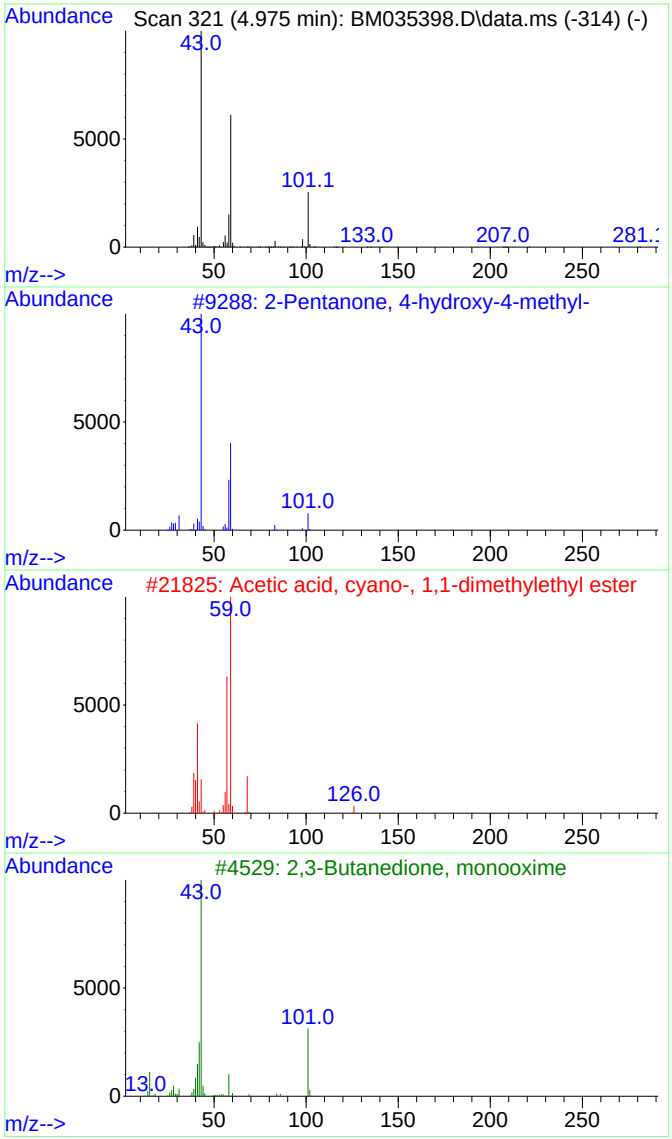
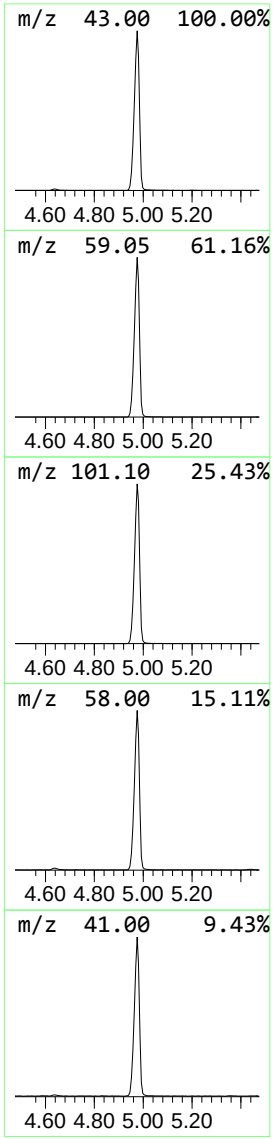
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	152.91 ng	6674200	1,4-Dichlorobenzene-d4	7.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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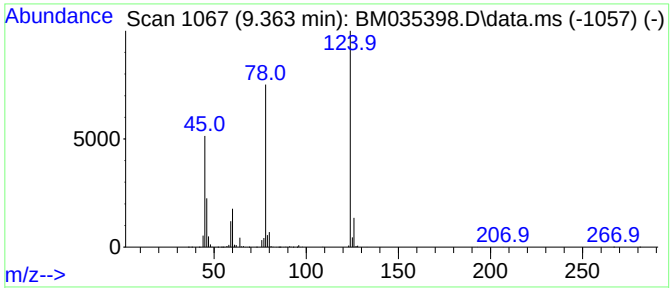
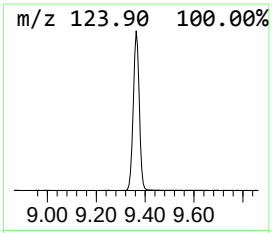
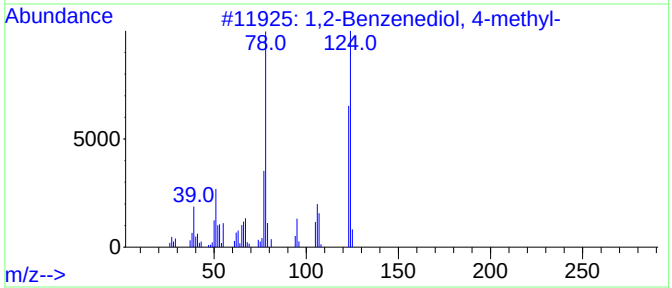
****
Peak Number 2 1,2-Benzenediol, 4-methyl- Concentration Rank 2

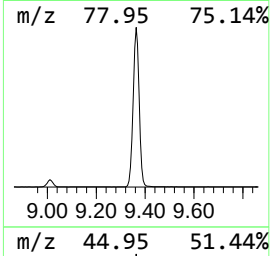
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.363	35.19 ng	2088410	Naphthalene-d8	10.645

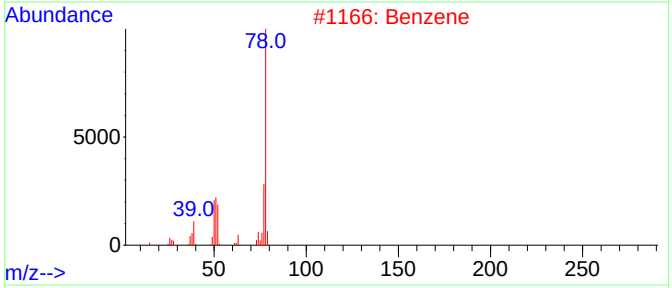
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	50
2	Benzene	78	C6H6	000071-43-2	9
3	Fumaronitrile	78	C4H2N2	000764-42-1	9
4	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	9
5	Propanedinitrile, methylene-	78	C4H2N2	000922-64-5	7

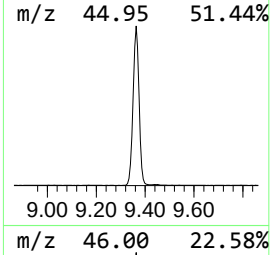


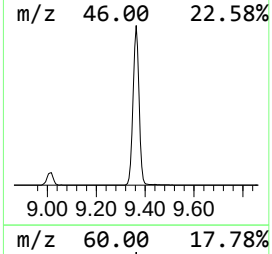


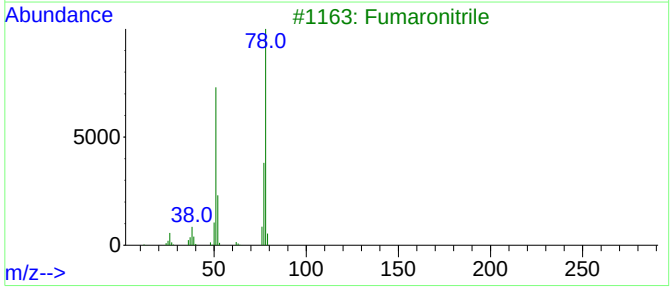


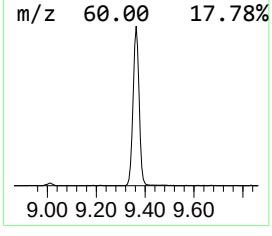












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

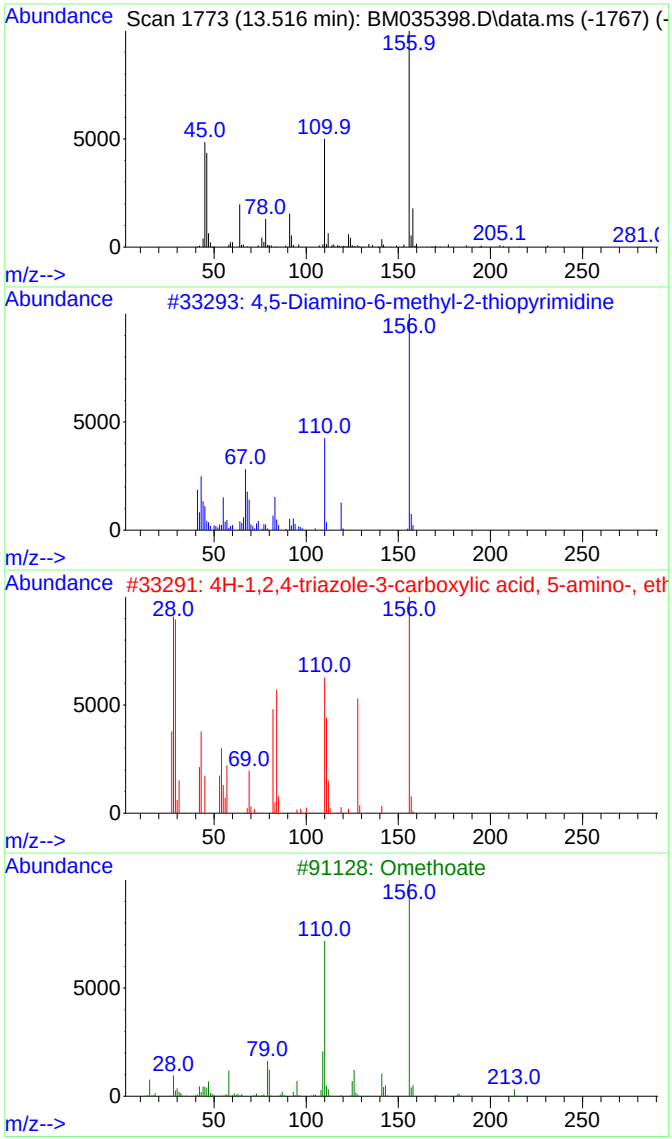
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

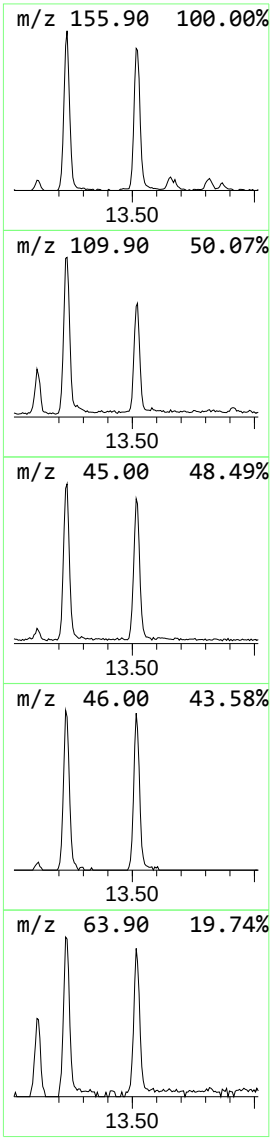
****

Peak Number 3 unknown13.516 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.516	2.24 ng	192162	Acenaphthene-d10	14.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5-Diamino-6-methyl-2-thiopyrim...	156	C5H8N4S	006305-99-3	47
2	4H-1,2,4-triazole-3-carboxylic a...	156	C5H8N4O2	1000404-32-7	32
3	Omethoate	213	C5H12NO4PS	001113-02-6	25
4	[1,2,3,4]Tetrathiane	156	C2H4S4	000290-81-3	17
5	Orotyl-2,2-dimethylhydrazide	198	C7H10N4O3	1000250-76-4	10





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TIC Library : C:\Database\NIST20.L
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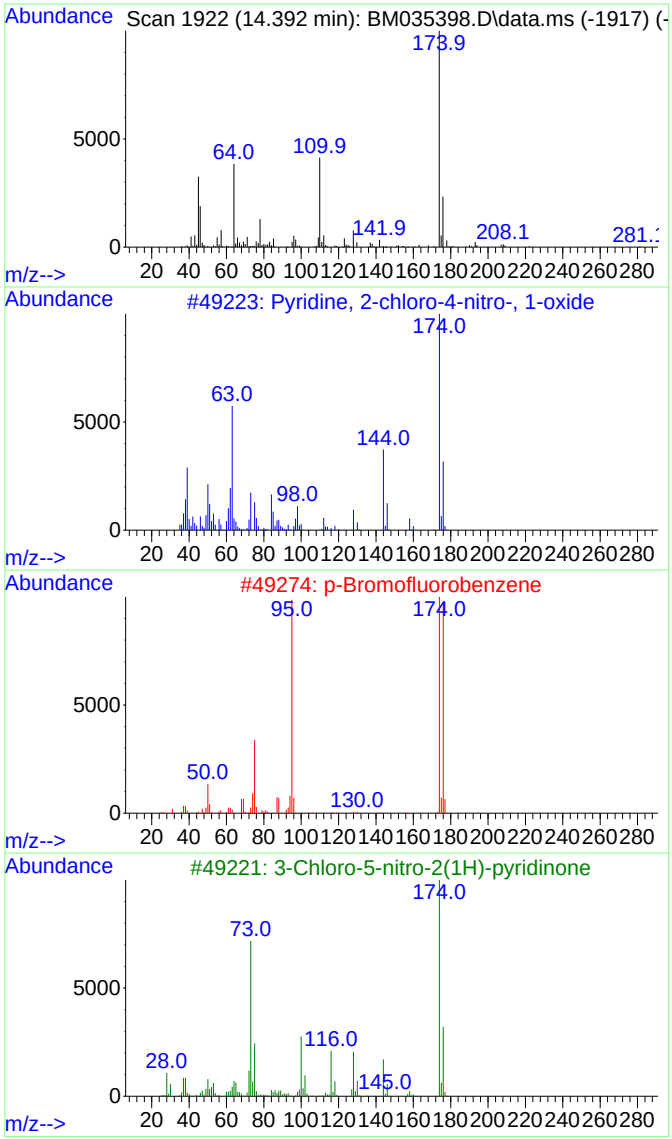
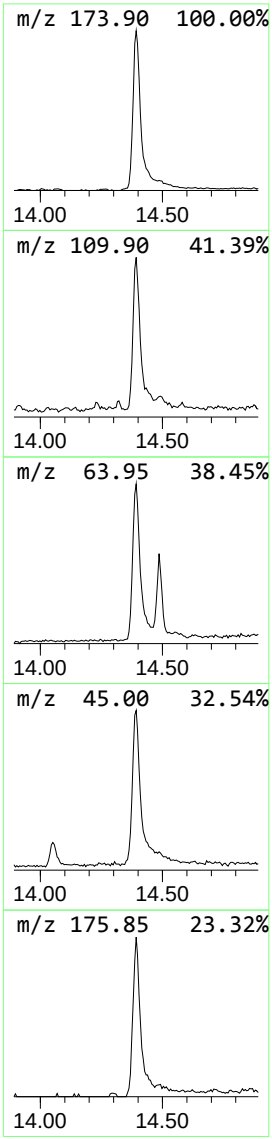
Peak Number 4 unknown14.392 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	3.20 ng	274483	Acenaphthene-d10	14.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-chloro-4-nitro-, 1-o...	174	C5H3ClN2O3	014432-16-7	10
2	p-Bromofluorobenzene	174	C6H4BrF	000460-00-4	9
3	3-Chloro-5-nitro-2(1H)-pyridinone	174	C5H3ClN2O3	022353-38-4	9
4	Benzene, 1-bromo-3-fluoro-	174	C6H4BrF	001073-06-9	9
5	2,4-Dinitrothiophene	174	C4H2N2O4S	005347-12-6	9





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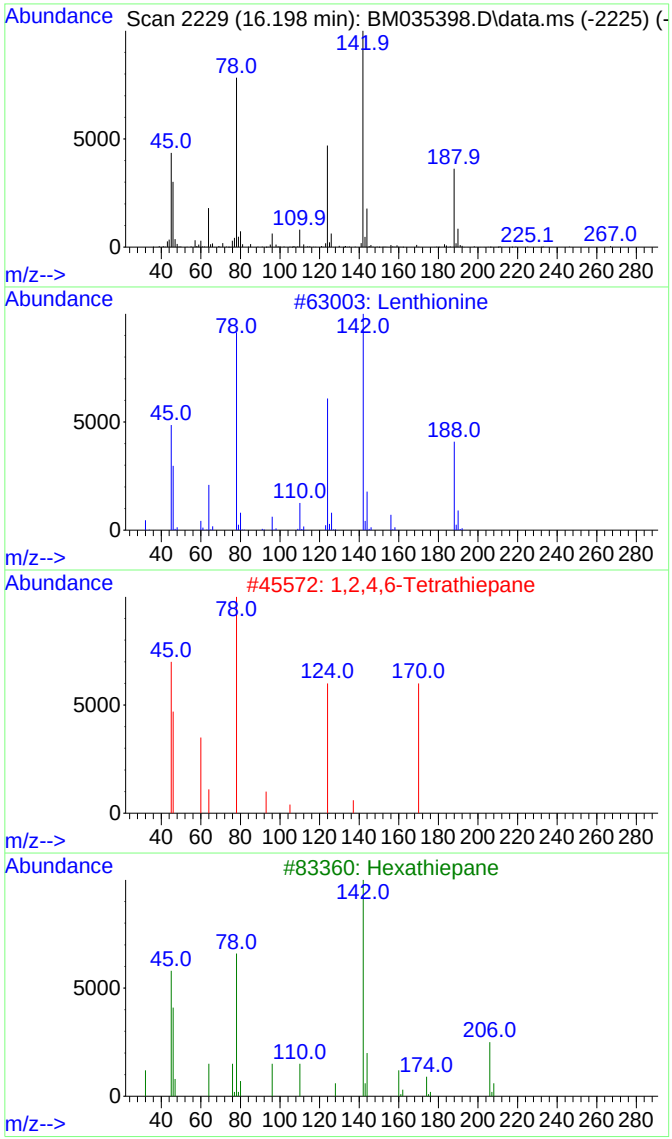
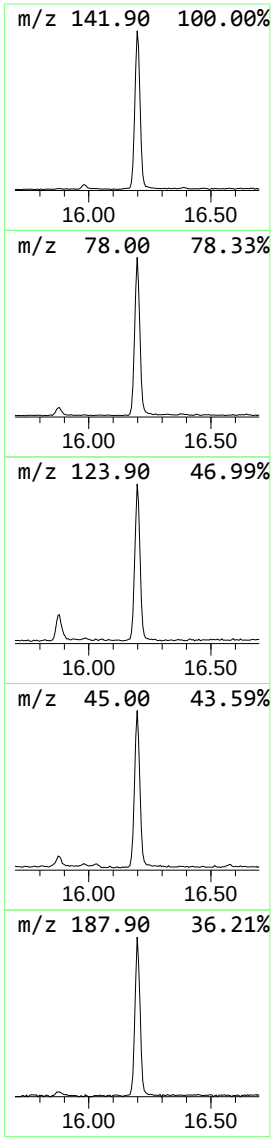
Peak Number 5 Lenthionine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.198	4.90 ng	455191	Phenanthrene-d10	17.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	93
2	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
3	Hexathiepane	206	CH2S6	017233-71-5	40
4	Ehylthiophosphonamide, o-methyl ...	139	C3H10NOPS	1000306-03-7	33
5	4-Chloro-2-nitrobenzyl alcohol	187	C7H6ClNO3	022996-18-5	25





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TIC Library : C:\Database\NIST20.L
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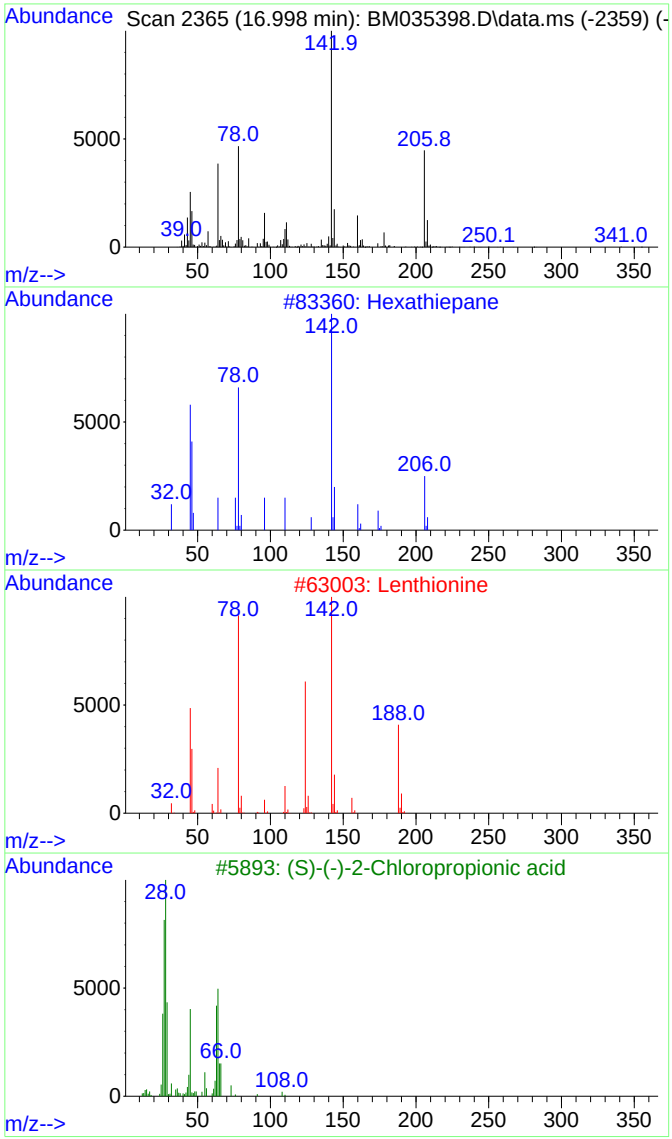
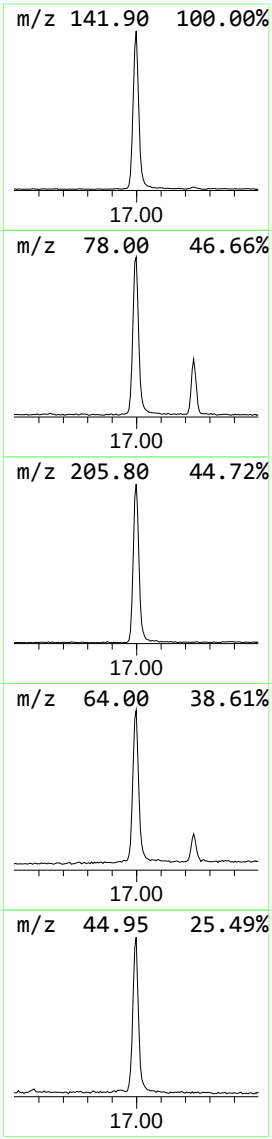
Peak Number 6 unknown16.998 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.998	8.07 ng	749639	Phenanthrene-d10	17.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiepane	206	CH2S6	017233-71-5	32
2	Lenthionine	188	C2H4S5	000292-46-6	14
3	(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	12
4	1,3-Benzenedithiol	142	C6H6S2	000626-04-0	10
5	L-Leucine, N-(n-butyl)-, methyl ...	201	C11H23NO2	1000452-94-2	9





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TIC Library : C:\Database\NIST20.L
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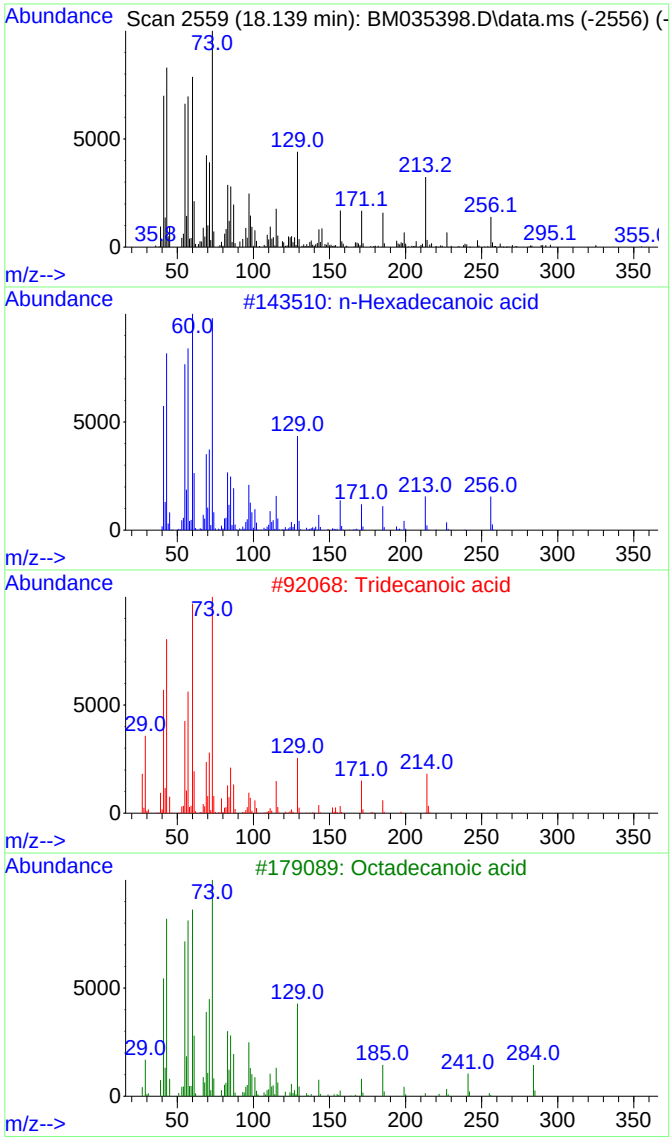
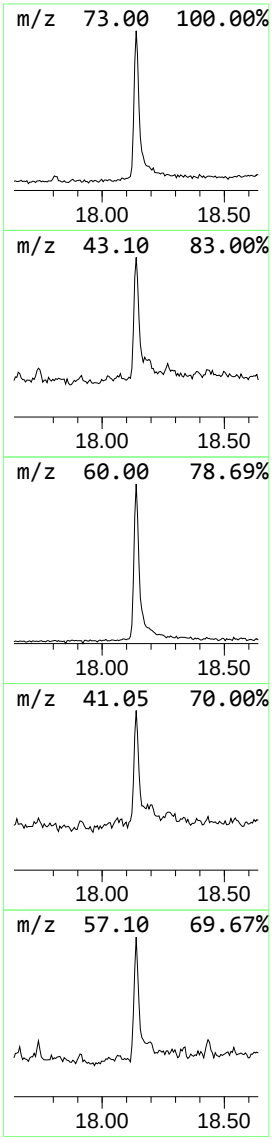
Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	3.18 ng	295888	Phenanthrene-d10	17.233

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	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

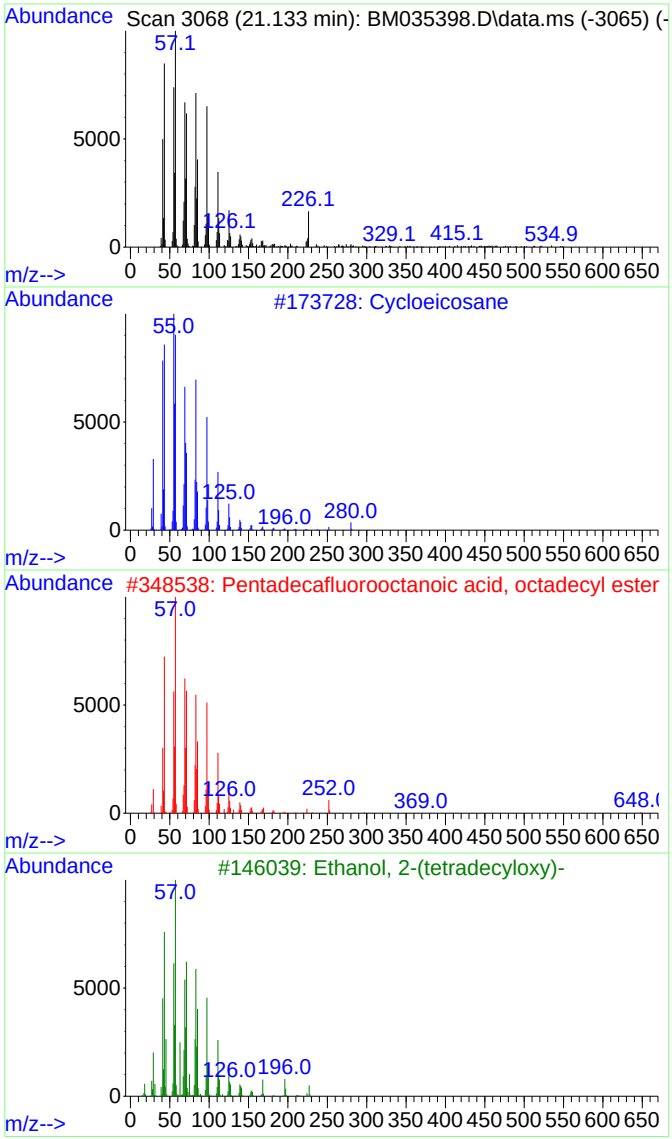
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

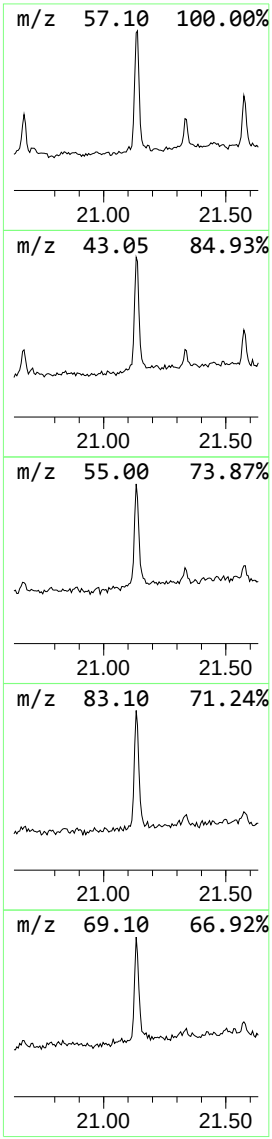
****

Peak Number 8 Cycloeicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	3.49 ng	470406	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	95
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	94
4	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060322\
Data File : BM035398.D
Acq On : 03 Jun 2022 16:56
Operator : CG/JU
Sample : N3143-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20220425-AMENDED-COMP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.975	152.9	ng	6674200	1	7.845	872950	20.0
1,2-Benzenediol...	9.363	35.2	ng	2088410	2	10.645	1186960	20.0
unknown13.516	13.516	2.2	ng	192162	3	14.486	1715010	20.0
unknown14.392	14.392	3.2	ng	274483	3	14.486	1715010	20.0
Lenthionine	16.198	4.9	ng	455191	4	17.233	1858330	20.0
unknown16.998	16.998	8.1	ng	749639	4	17.233	1858330	20.0
n-Hexadecanoic ...	18.139	3.2	ng	295888	4	17.233	1858330	20.0
Cycloeicosane	21.133	3.5	ng	470406	5	21.421	2693710	20.0