LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036193.D
Acq On : 10 Aug 2022 15:39
Operator : CG/JU
Sample : N3971-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-15

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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.281	198	203	214	rBV	862046	1176661	9.60%	1.979%
2	4.922	307	312	320	rBV2	301854	469671	3.83%	0.790%
3	5.322	374	380	384	rBV	93879	142849	1.17%	0.240%
4	5.416	390	396	412	rVB	2079450	2957929	24.14%	4.974%
5	6.475	570	576	586	rVB	360241	513544	4.19%	0.864%
6	6.887	638	646	652	rBV	95915	164425	1.34%	0.276%
7	7.034	664	671	682	rBV	1162415	1819759	14.85%	3.060%
8	7.834	800	807	813	rBV	867350	1354317	11.05%	2.277%
9	7.898	813	818	831	rVB	188685	337322	2.75%	0.567%
10	8.457	905	913	923	rBV	99879	178885	1.46%	0.301%
11	9.004	999	1006	1016	rBV	2614413	4130877	33.71%	6.946%
12	9.157	1025	1032	1040	rBV3	75258	165614	1.35%	0.278%
13	9.569	1097	1102	1109	rVB	152304	240718	1.96%	0.405%
14	9.992	1168	1174	1184	rVB	109273	194195	1.58%	0.327%
15	10.428	1238	1248	1256	rBV2	75367	145909	1.19%	0.245%
16	10.633	1276	1283	1291	rBV	1118723	1885073	15.38%	3.170%
17	11.016	1341	1348	1362	rBV	72180	167610	1.37%	0.282%
18	11.604	1443	1448	1464	rVB	109065	250485	2.04%	0.421%
19	12.839	1653	1658	1665	rBV2	83200	149772	1.22%	0.252%
20	12.927	1669	1673	1682	rVB2	62318	141260	1.15%	0.238%
21	13.104	1695	1703	1719	rBV	6096185	9154972	74.70%	15.395%
22	13.333	1735	1742	1756	rBV	2202790	3054861	24.93%	5.137%
23	14.474	1930	1936	1944	rVB	1639399	2309464	18.84%	3.884%
24	15.298	2068	2076	2082	rVB	84248	147753	1.21%	0.248%
25	15.833	2162	2167	2171	rBV	103314	134924	1.10%	0.227%
26	15.968	2183	2190	2199	rBV	4650642	6644670	54.22%	11.174%
27	17.215	2396	2402	2410	rBV	1829901	2549340	20.80%	4.287%
28	17.886	2511	2516	2522	rVB	203767	252713	2.06%	0.425%
29	18.115	2551	2555	2564	rBV	152890	243876	1.99%	0.410%
30	19.845	2843	2849	2854	rBV	10131138	12255163	100.00%	20.608%
31	21.397	3108	3113	3123	rBV	2382695	2985628	24.36%	5.021%
32	23.744	3506	3512	3524	rVB2	1574691	3147161	25.68%	5.292%

Sum of corrected areas: 59467400

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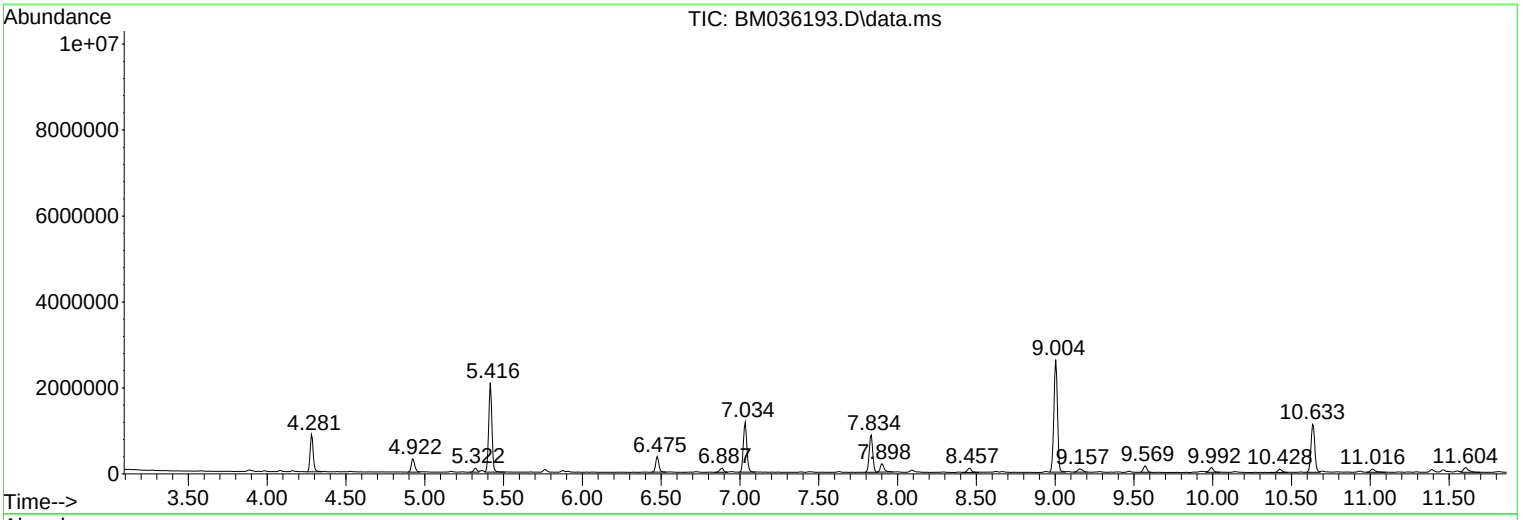
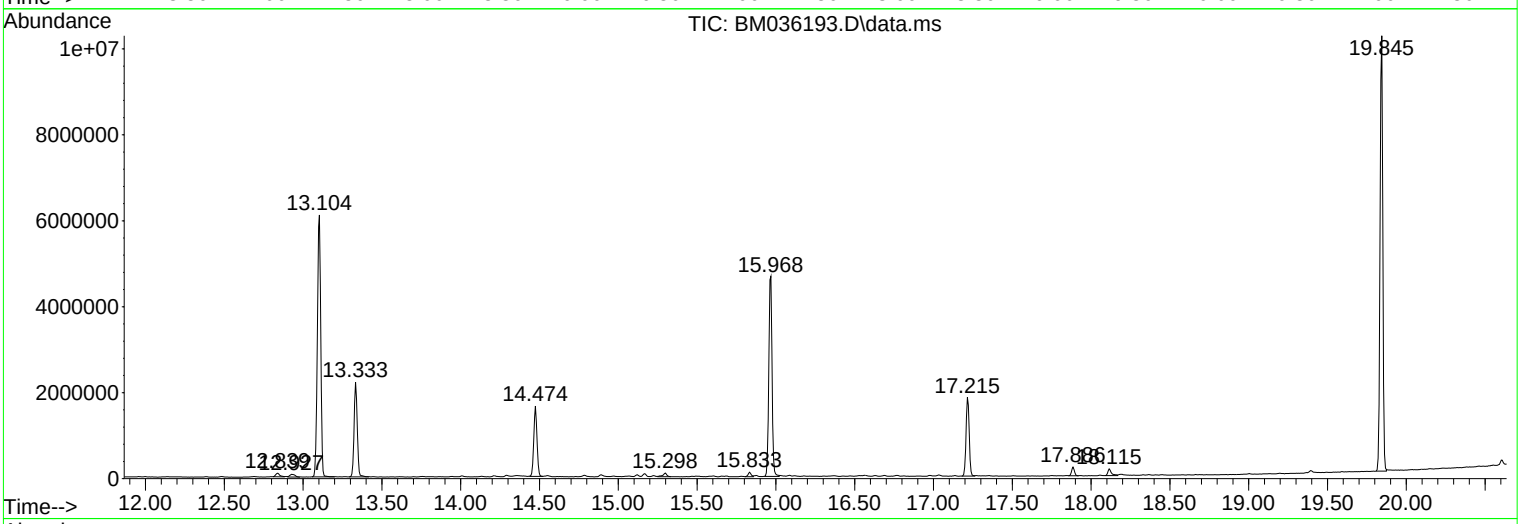
Misc :
ALS Vial : 8 Sample Multiplier: 1

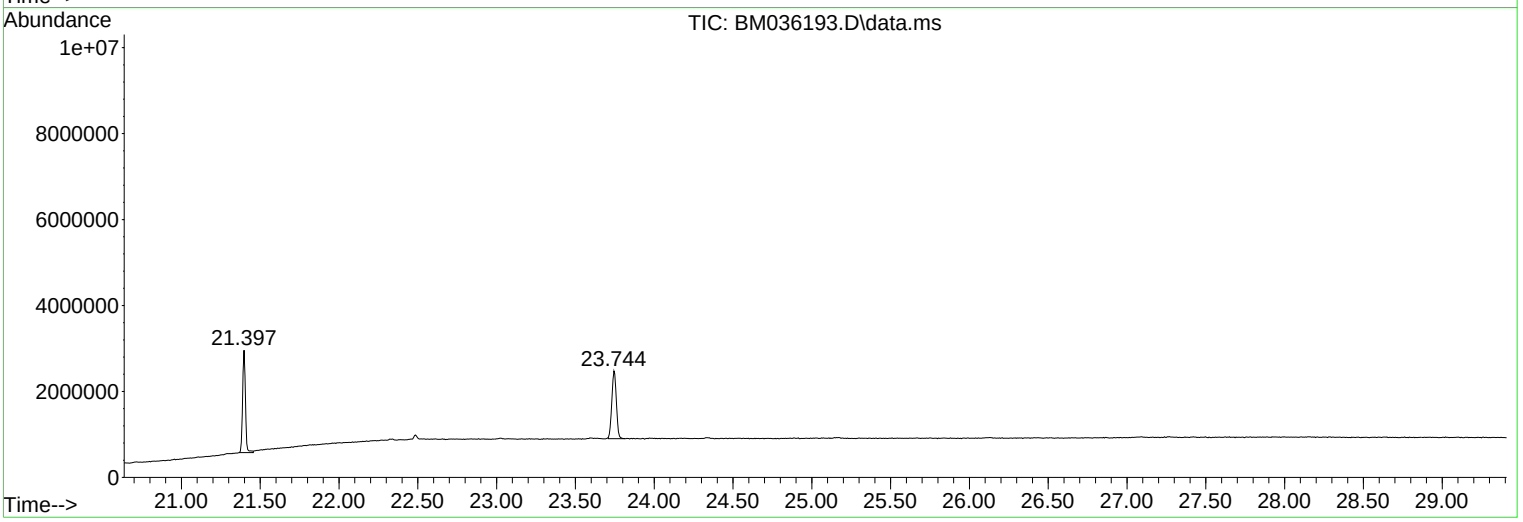
Instrument :
BNA_M
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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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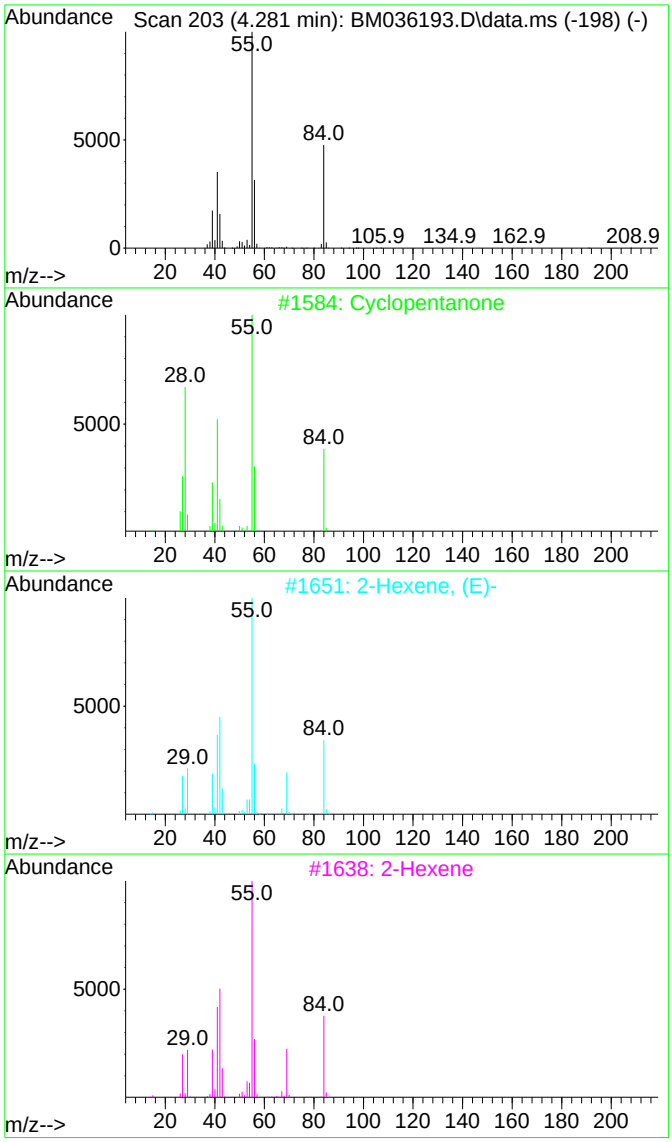
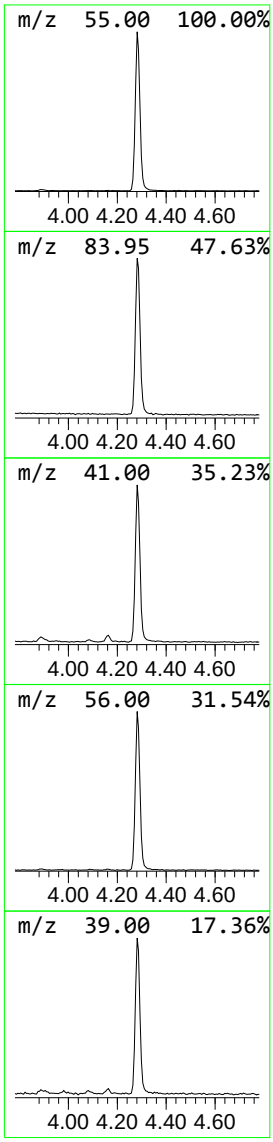
****

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.281	17.38 ng	1176660	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene, (E)-	84	C6H12	004050-45-7	64
3	2-Hexene	84	C6H12	000592-43-8	59
4	3-Hexene, (Z)-	84	C6H12	007642-09-3	59
5	2(5H)-Furanone	84	C4H4O2	000497-23-4	52





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TIC Library : C:\Database\NIST20.L
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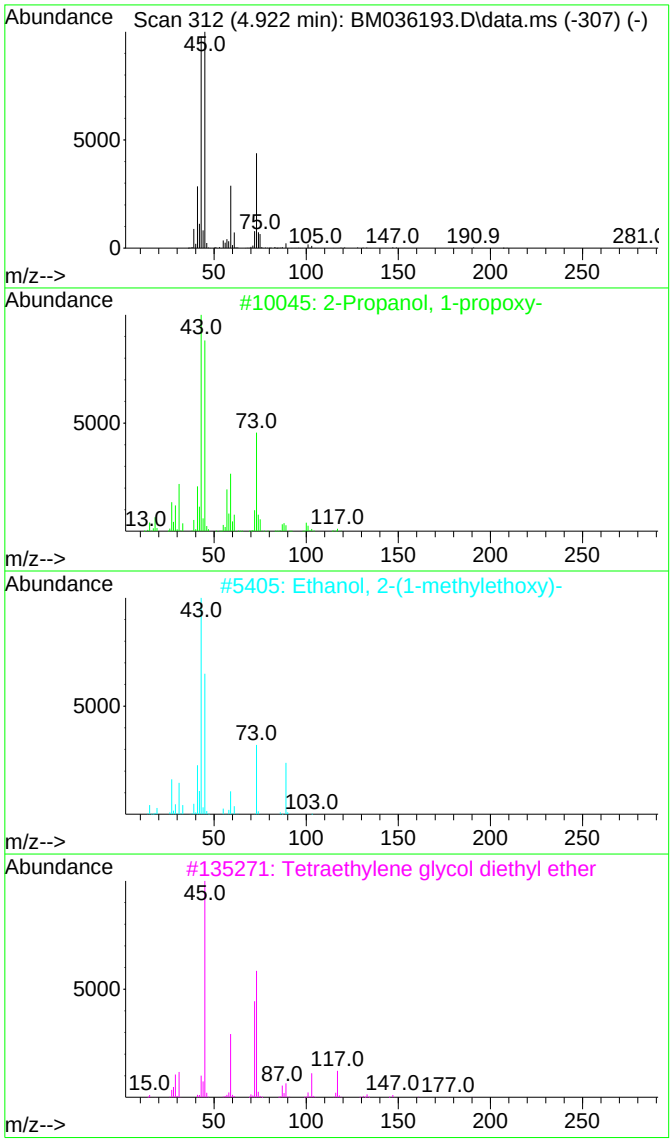
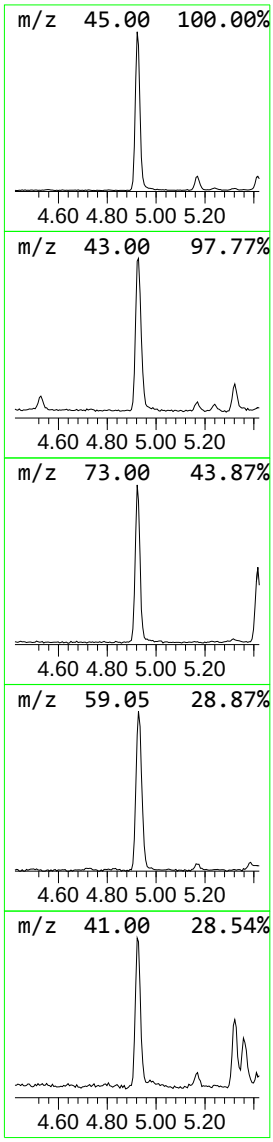
****
Peak Number 2 2-Propanol, 1-propoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	6.94 ng	469671	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	74
2	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	72
3	Tetraethylene glycol diethyl ether	250	C12H26O5	004353-28-0	53
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
5	2-Butanol	74	C4H10O	000078-92-2	50





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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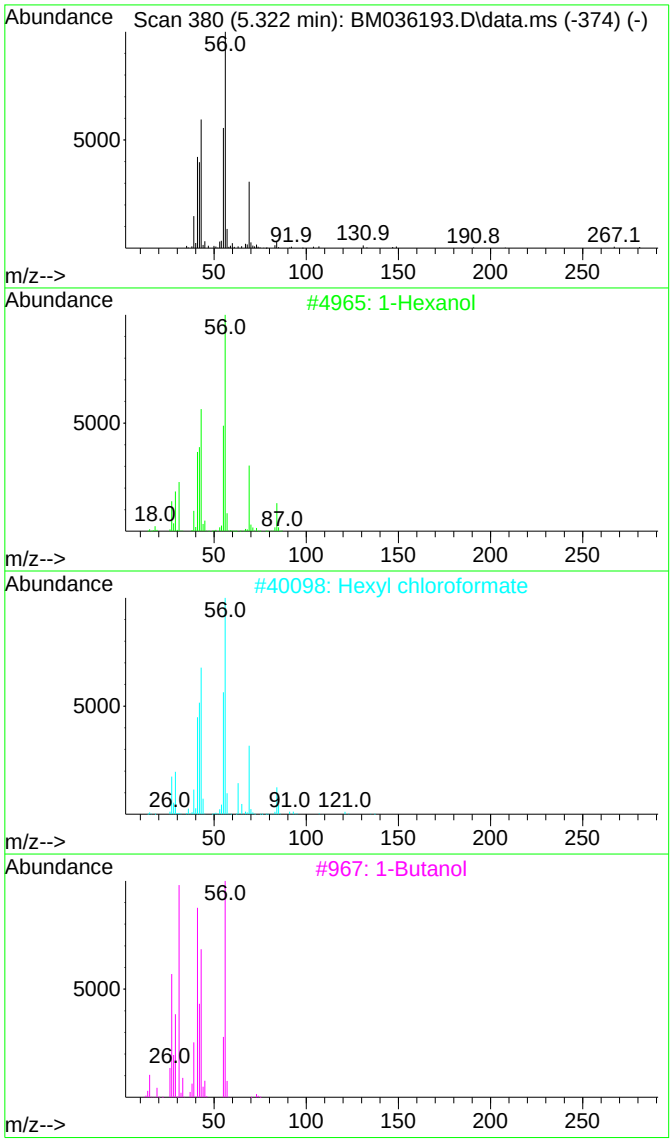
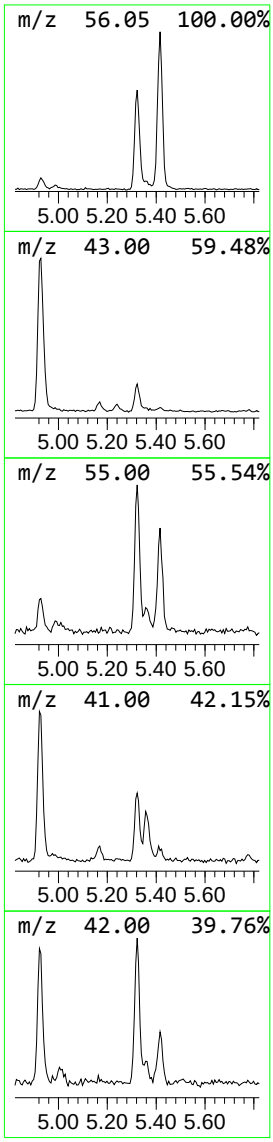
Peak Number 3 1-Hexanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.322	2.11 ng	142849	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	78
2	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
3	1-Butanol	74	C4H10O	000071-36-3	72
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	64
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	53





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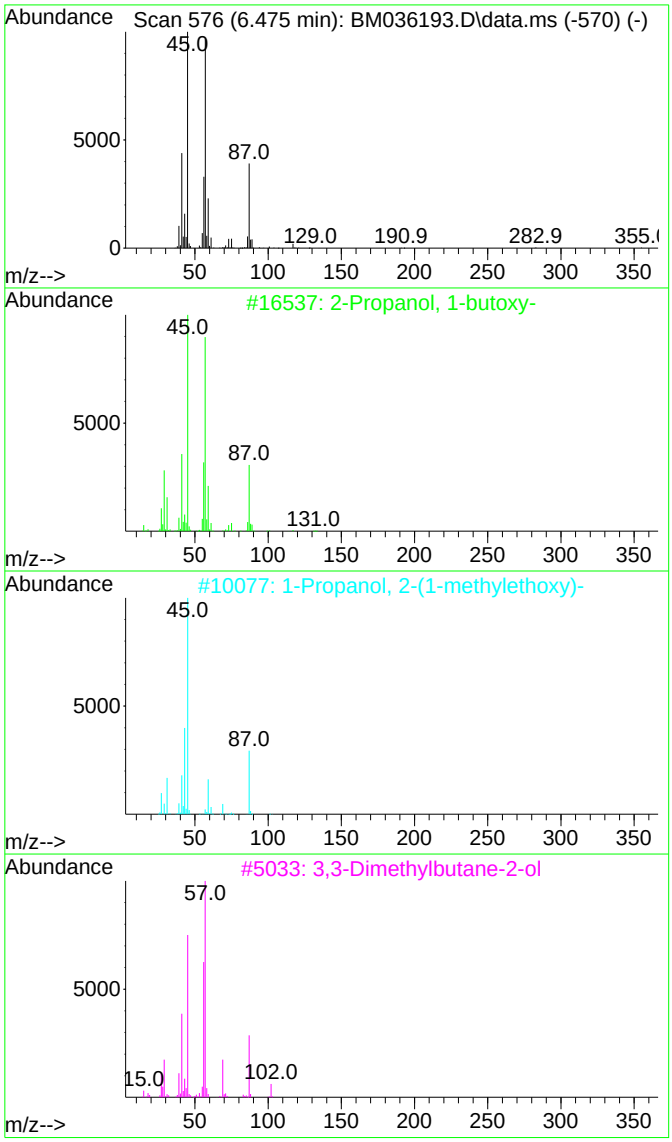
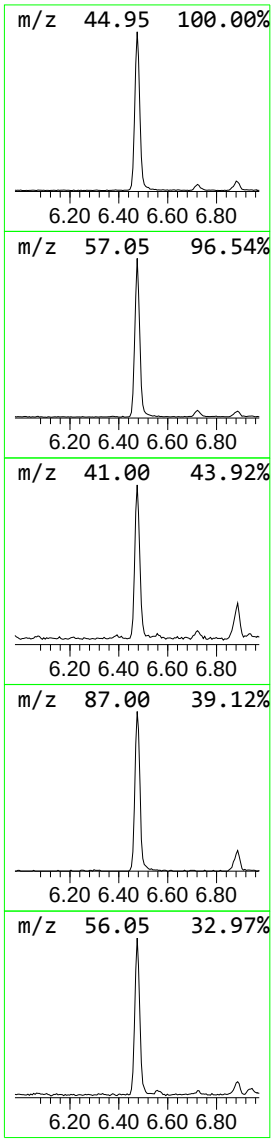
Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.475	7.58 ng	513544	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	53
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
4	Diisopropyl ether	102	C6H14O	000108-20-3	42
5	5-Methyl-1-hepten-4-ol	128	C8H16O	099328-46-8	40





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
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TIC Library : C:\Database\NIST20.L
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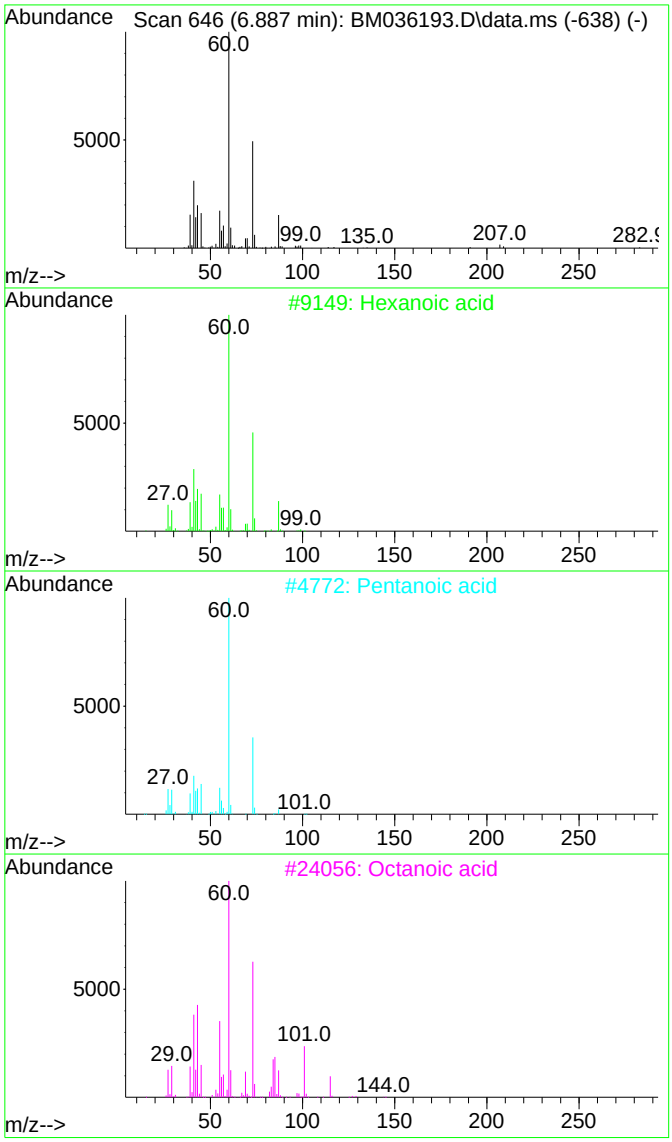
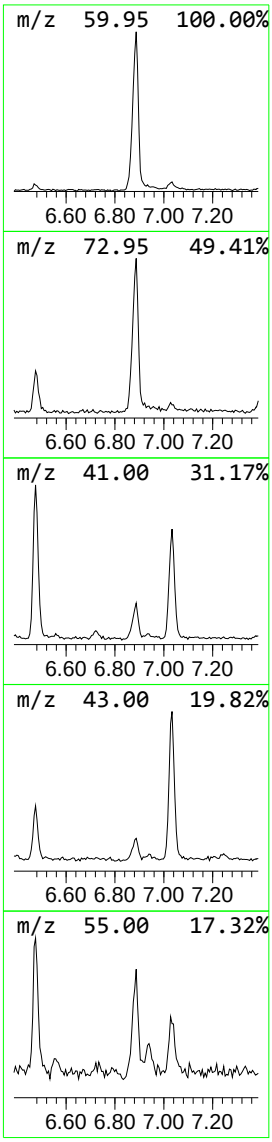
Peak Number 5 Hexanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.887	2.43 ng	164425	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	90
2	Pentanoic acid	102	C5H10O2	000109-52-4	72
3	Octanoic acid	144	C8H16O2	000124-07-2	64
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
5	Heptanoic acid	130	C7H14O2	000111-14-8	56





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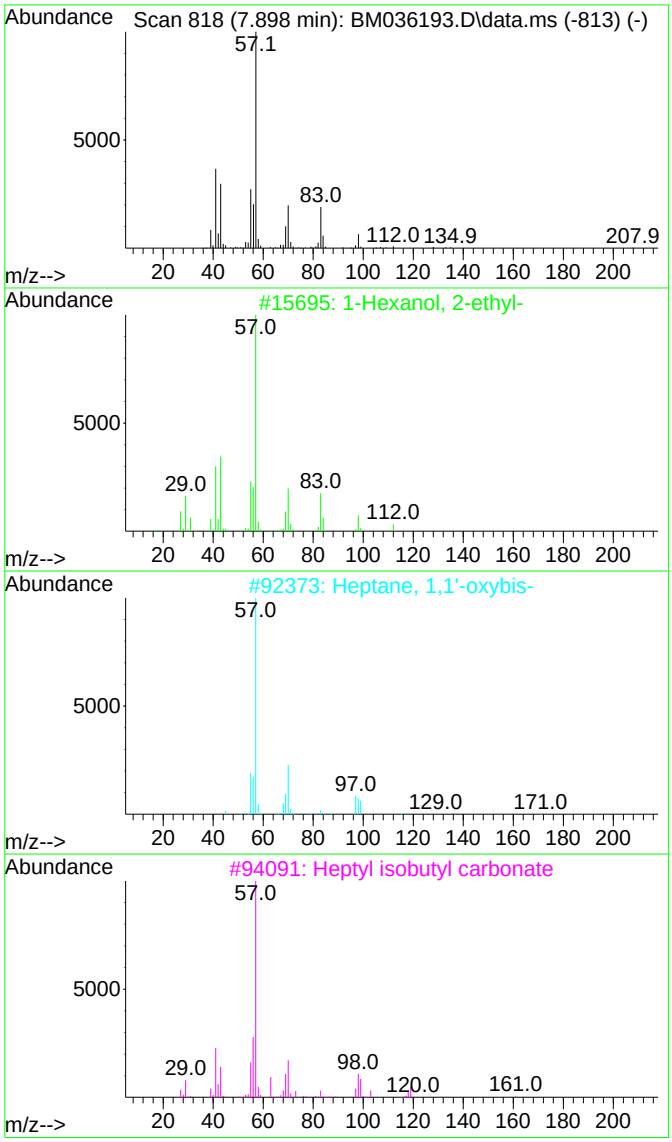
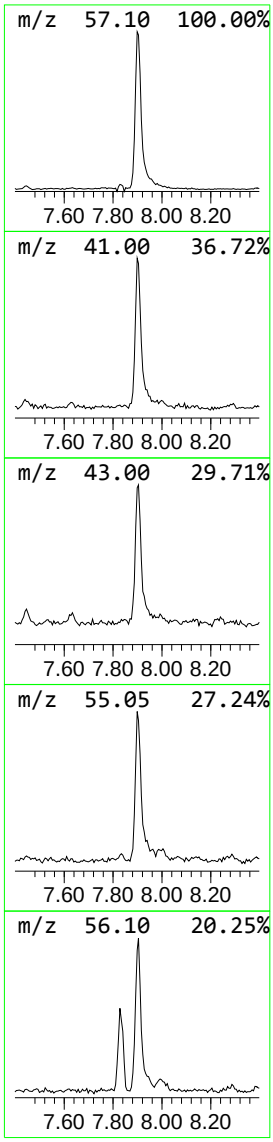
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	4.98 ng	337322	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	59
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50





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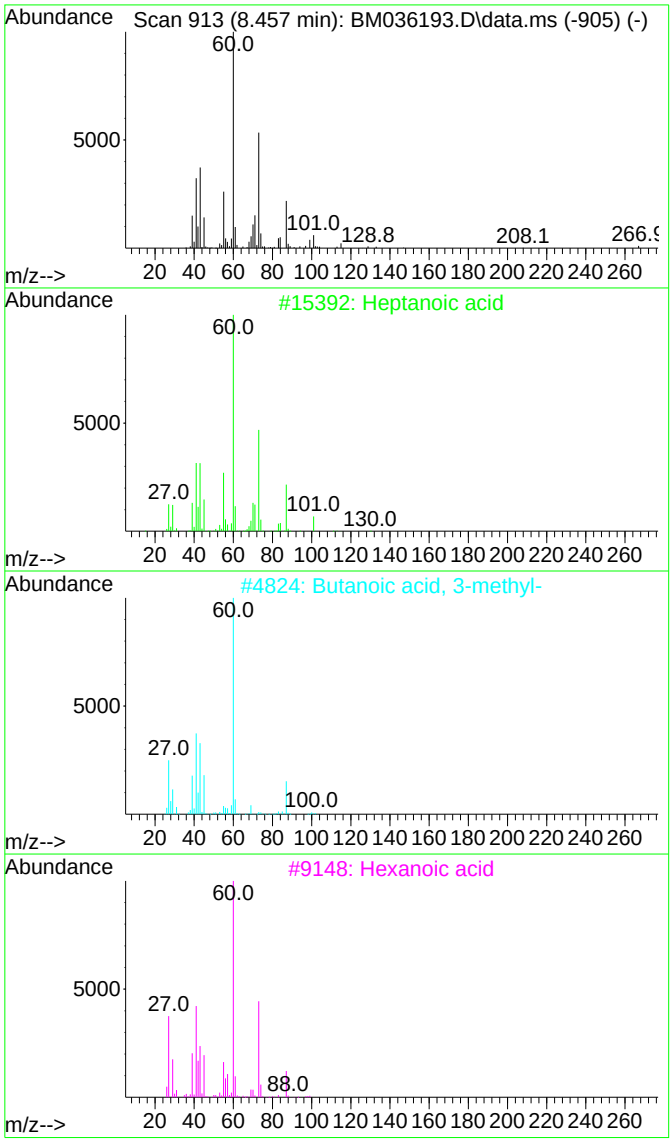
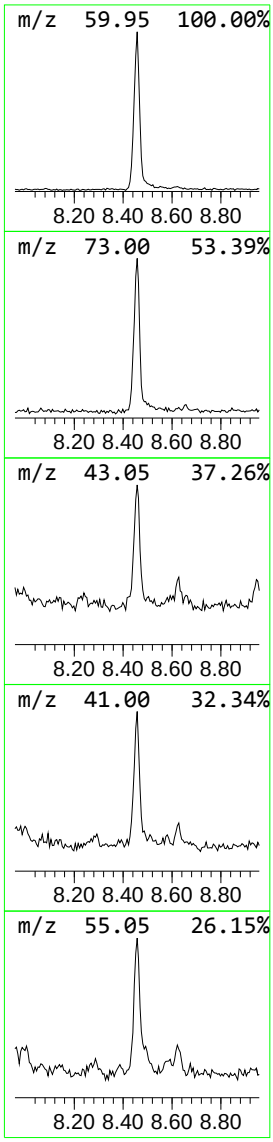
****

Peak Number 7 Heptanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	2.64 ng	178885	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	91
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	58
3	Hexanoic acid	116	C6H12O2	000142-62-1	50
4	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	50
5	Pentanoic acid	102	C5H10O2	000109-52-4	50





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TIC Library : C:\Database\NIST20.L
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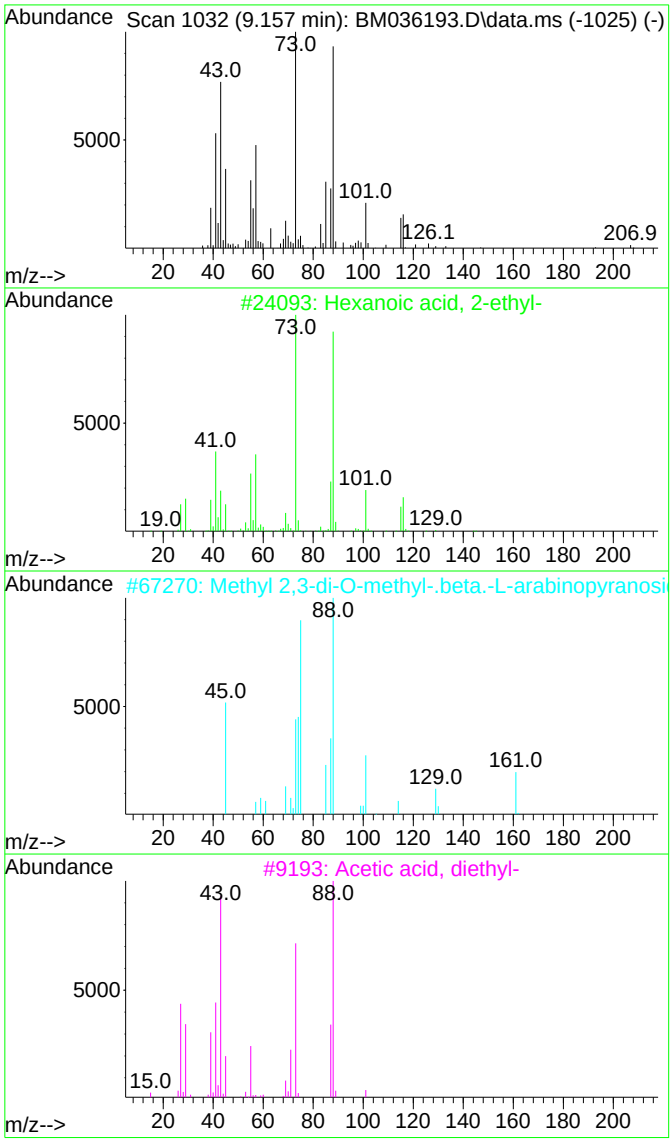
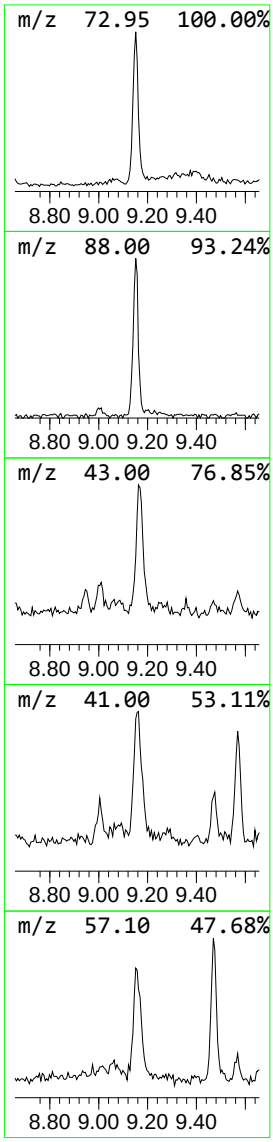
****
Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	2.45 ng	165614	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	64
2	Methyl 2,3-di-O-methyl-.beta.-L-...	192	C8H16O5	053989-92-7	64
3	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	47
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	43
5	Hydrazine, 1-methyl-1-(1-methyle...	88	C4H12N2	033668-54-1	43





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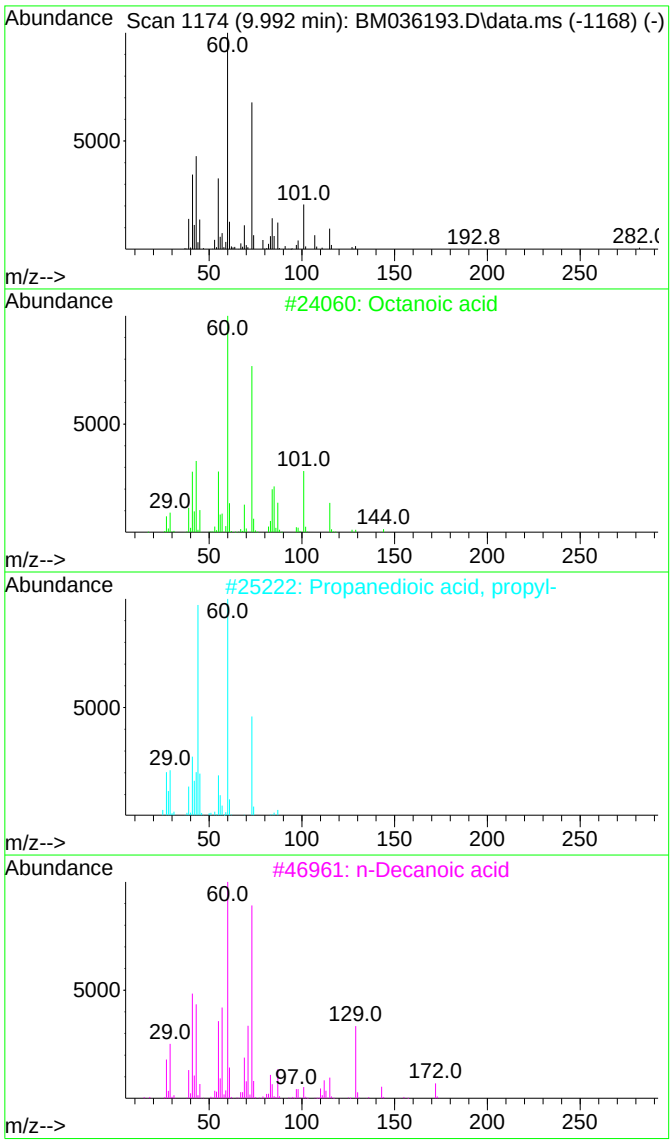
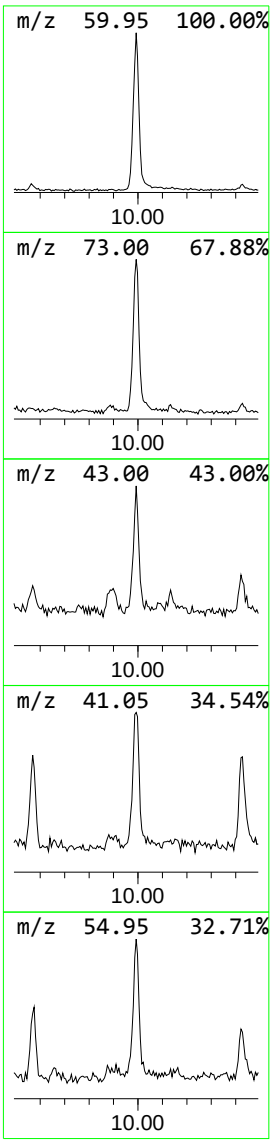
Peak Number 9 Octanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.992	2.06 ng	194195	Naphthalene-d8	10.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	86
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Pentanoic acid	102	C5H10O2	000109-52-4	50
5	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036193.D
Acq On : 10 Aug 2022 15:39
Operator : CG/JU
Sample : N3971-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-15

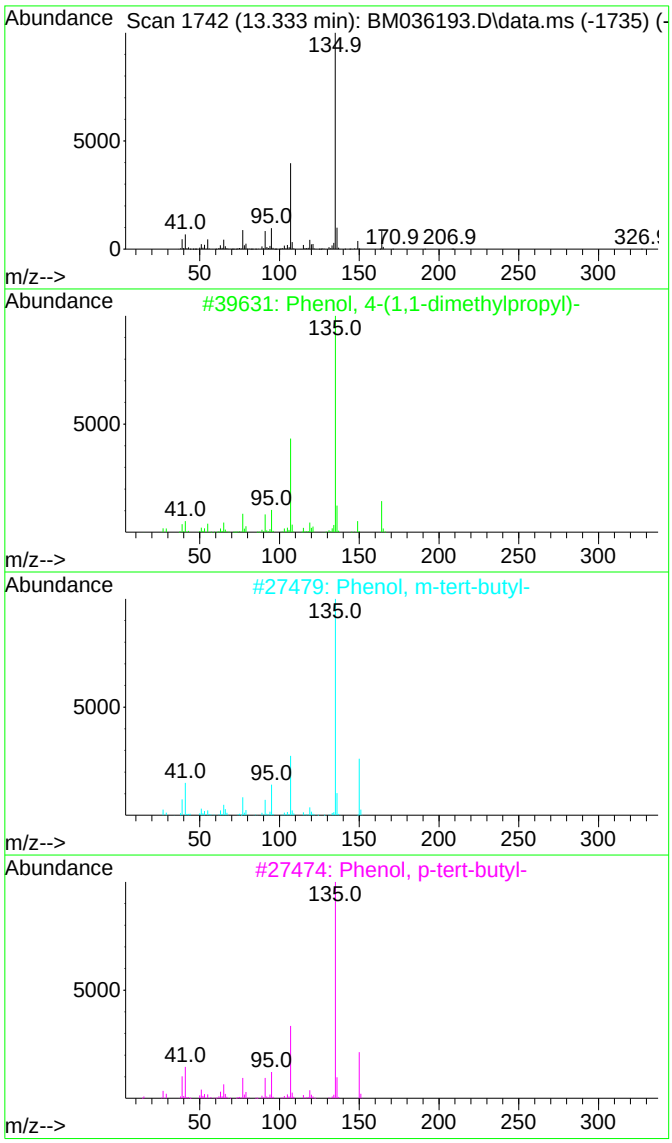
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

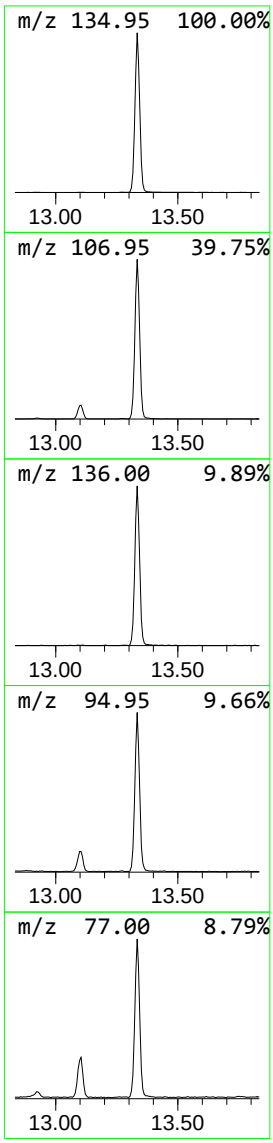
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	26.46 ng	3054860	Acenaphthene-d10	14.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	86
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5	4,6-Bis(4-ethoxybenzylthio)-5-ni...	457	C22H23N3O4S2	325957-76-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036193.D
Acq On : 10 Aug 2022 15:39
Operator : CG/JU
Sample : N3971-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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
Cyclopentanone	4.281	17.4	ng	1176660	1	7.834	1354320	20.0
2-Propanol, 1-p...	4.922	6.9	ng	469671	1	7.834	1354320	20.0
1-Hexanol	5.322	2.1	ng	142849	1	7.834	1354320	20.0
2-Propanol, 1-b...	6.475	7.6	ng	513544	1	7.834	1354320	20.0
Hexanoic acid	6.887	2.4	ng	164425	1	7.834	1354320	20.0
1-Hexanol, 2-et...	7.898	5.0	ng	337322	1	7.834	1354320	20.0
Heptanoic acid	8.457	2.6	ng	178885	1	7.834	1354320	20.0
Hexanoic acid, ...	9.157	2.5	ng	165614	1	7.834	1354320	20.0
Octanoic acid	9.992	2.1	ng	194195	2	10.634	1885070	20.0
Phenol, 4-(1,1-...	13.333	26.5	ng	3054860	3	14.474	2309460	20.0