LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036197.D
Acq On : 10 Aug 2022 18:09
Operator : CG/JU
Sample : N3972-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-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: BM036197.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	rVB	1010937	1362372	12.08%	2.328%
2	4.922	307	312	319	rBV2	332781	510030	4.52%	0.871%
3	5.322	374	380	384	rBV	101542	152648	1.35%	0.261%
4	5.416	390	396	411	rVB	2063962	2979364	26.41%	5.090%
5	6.475	567	576	585	rBV	379378	557952	4.95%	0.953%
6	6.881	639	645	652	rBV	86174	146906	1.30%	0.251%
7	7.028	664	670	685	rBV	1139824	1820124	16.13%	3.110%
8	7.828	799	806	813	rBV	909837	1445536	12.81%	2.470%
9	7.898	813	818	826	rVV	122068	201107	1.78%	0.344%
10	8.093	844	851	864	rBV	91718	184511	1.64%	0.315%
11	8.457	906	913	927	rBV	135000	259316	2.30%	0.443%
12	9.004	998	1006	1017	rBV	2652671	4248066	37.65%	7.257%
13	9.569	1095	1102	1109	rBV	171732	271486	2.41%	0.464%
14	9.992	1165	1174	1188	rVB	161761	304077	2.70%	0.519%
15	10.634	1276	1283	1291	rBV	1192534	1966075	17.43%	3.359%
16	11.016	1342	1348	1361	rBV	51087	128800	1.14%	0.220%
17	11.386	1405	1411	1418	rBV2	57992	115139	1.02%	0.197%
18	11.469	1419	1425	1429	rBV	82240	128047	1.13%	0.219%
19	11.598	1440	1447	1465	rVB	343898	730519	6.47%	1.248%
20	13.104	1693	1703	1718	rBV	6096973	9025334	80.00%	15.419%
21	13.333	1734	1742	1749	rBV	1955467	2738541	24.27%	4.679%
22	14.210	1886	1891	1902	rBV	80704	144172	1.28%	0.246%
23	14.475	1928	1936	1944	rBV	1608675	2369304	21.00%	4.048%
24	15.963	2183	2189	2204	rBV	4472738	6266051	55.54%	10.705%
25	16.563	2286	2291	2298	rVB2	77547	125276	1.11%	0.214%
26	17.216	2396	2402	2409	rBV	1864944	2563393	22.72%	4.379%
27	17.886	2511	2516	2521	rVB2	216212	266586	2.36%	0.455%
28	19.845	2843	2849	2855	rBV	9274456	11282244	100.00%	19.275%
29	20.604	2975	2978	2983	rBV	123318	152593	1.35%	0.261%
30	21.398	3108	3113	3122	rBV	2337274	2982002	26.43%	5.095%
31	23.745	3506	3512	3523	rVB2	1617179	3106134	27.53%	5.307%

Sum of corrected areas: 58533705

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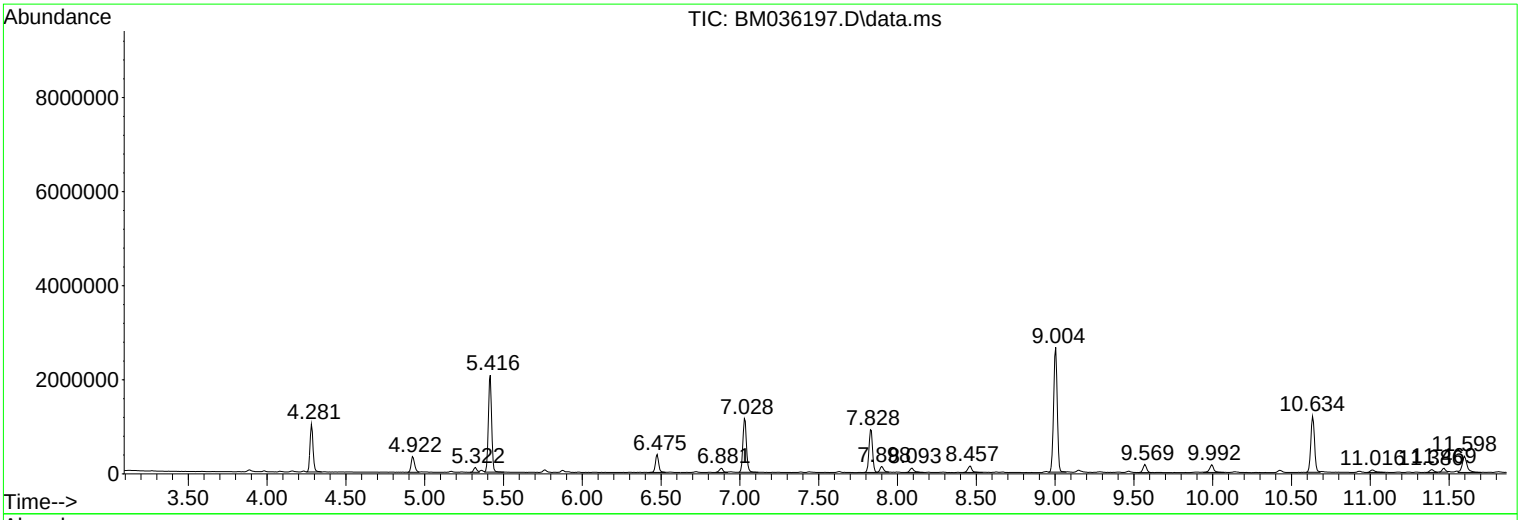
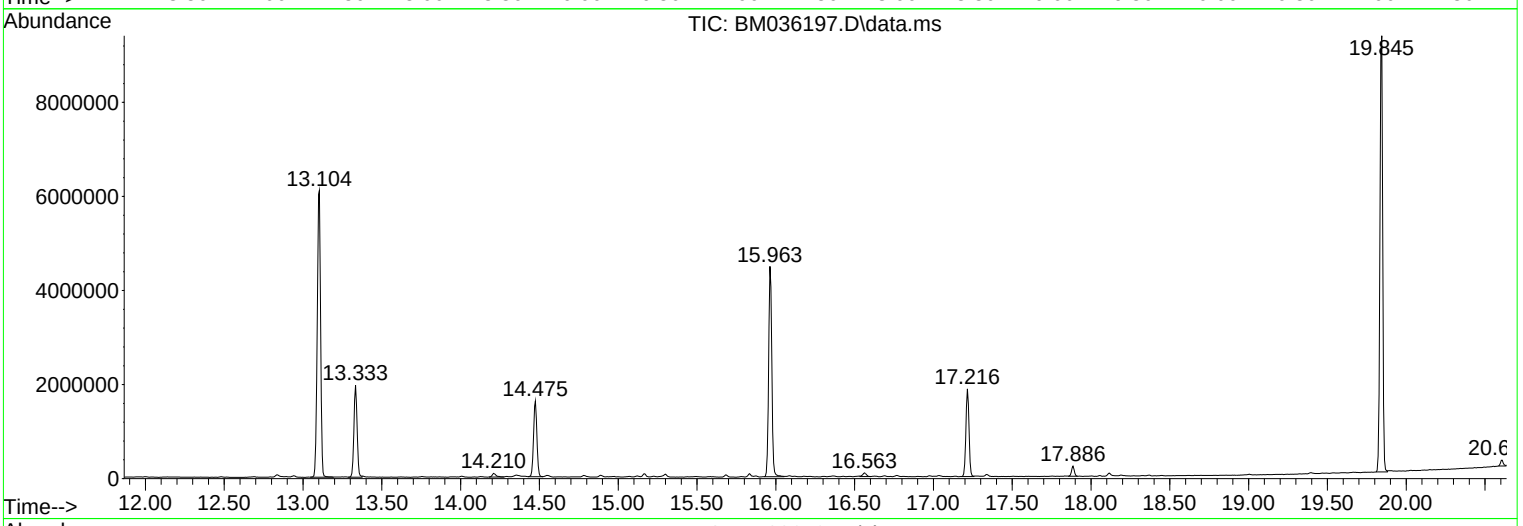
Sample : N3972-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

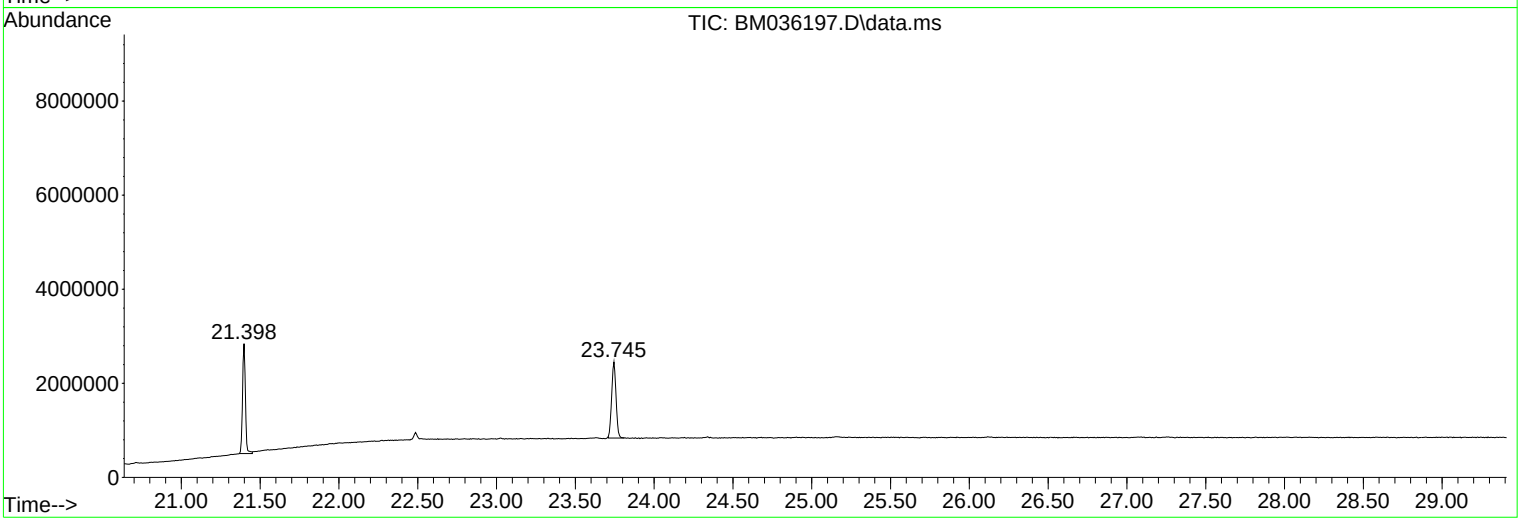
Instrument :
BNA_M
ClientSampleId :
SPN-15

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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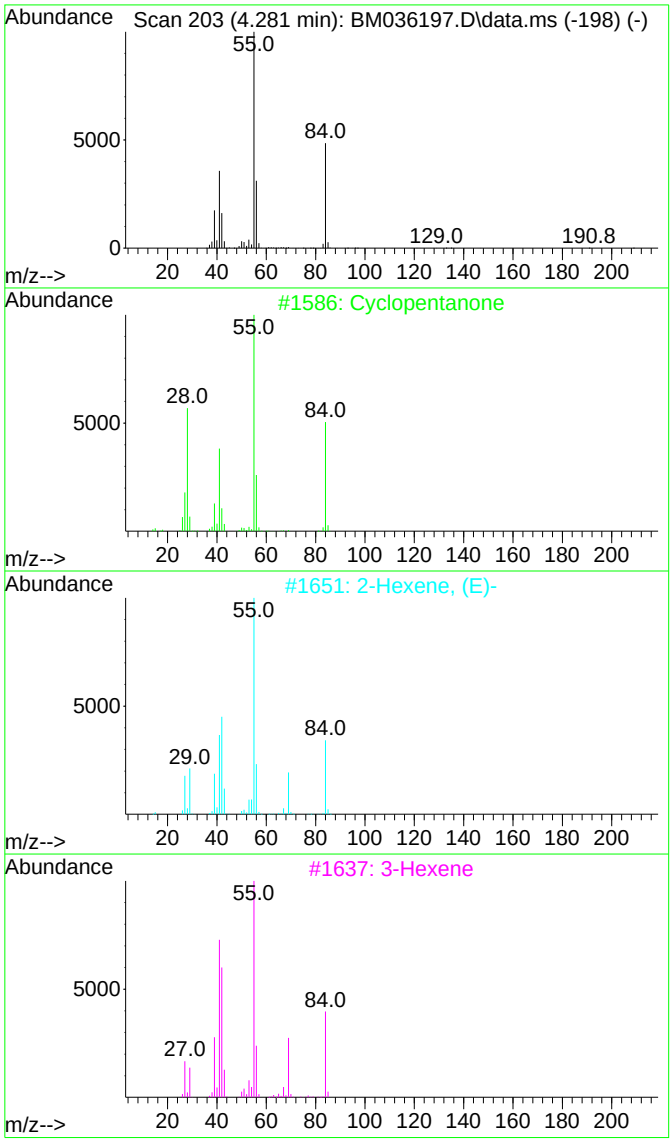
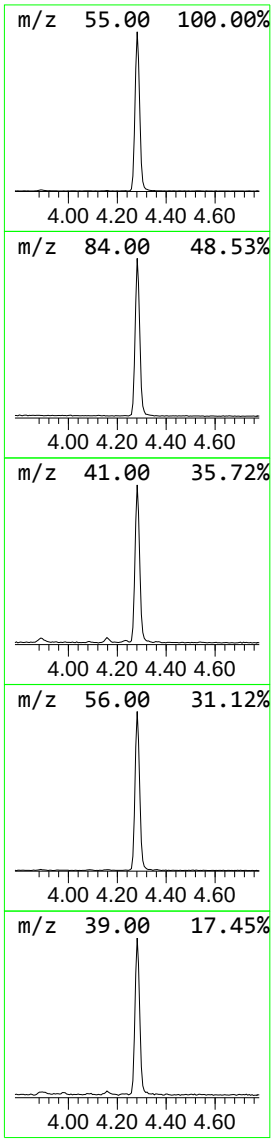
Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.281	18.85 ng	1362370	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	3-Hexene	84	C6H12	000592-47-2	45
4	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	45
5	2(5H)-Furanone	84	C4H4O2	000497-23-4	40





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Data File : BM036197.D
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Instrument :
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ClientSampleId :
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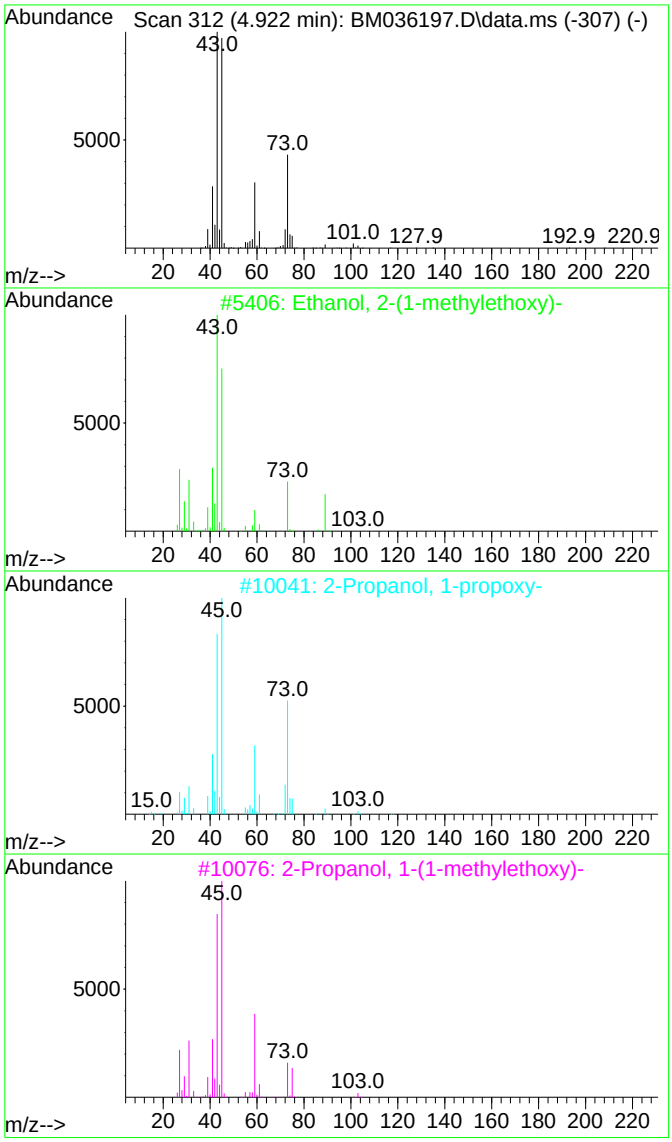
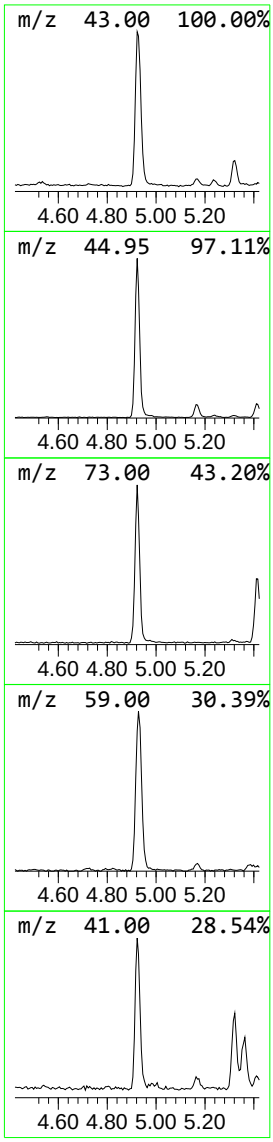
Peak Number 2 Ethanol, 2-(1-methylethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	7.06 ng	510030	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	78
2	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	78
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	56
4	Tetraethylene glycol diethyl ether	250	C12H26O5	004353-28-0	53
5	Sulfurous acid, bis(1-methylethy...	166	C6H14O3S	004773-13-1	50





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-15

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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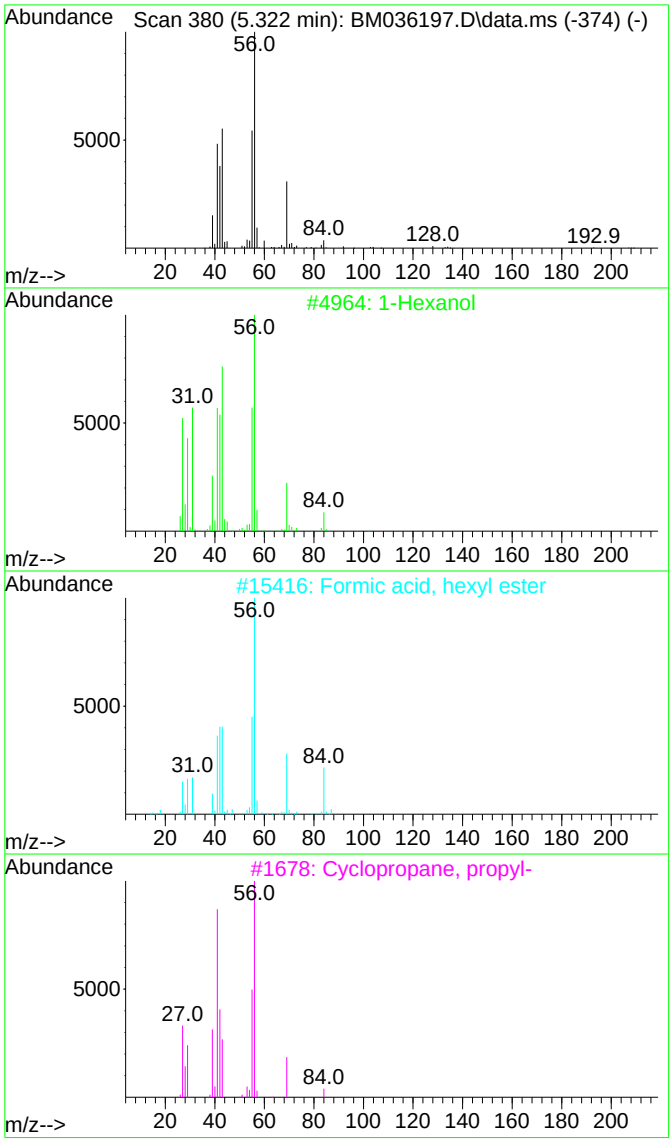
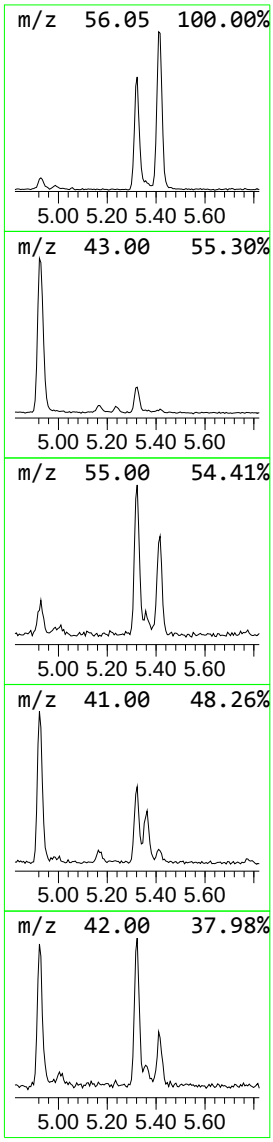
Peak Number 3 1-Hexanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.322	2.11 ng	152648	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
3	Cyclopropane, propyl-	84	C6H12	002415-72-7	78
4	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
5	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72





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Data File : BM036197.D
Acq On : 10 Aug 2022 18:09
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
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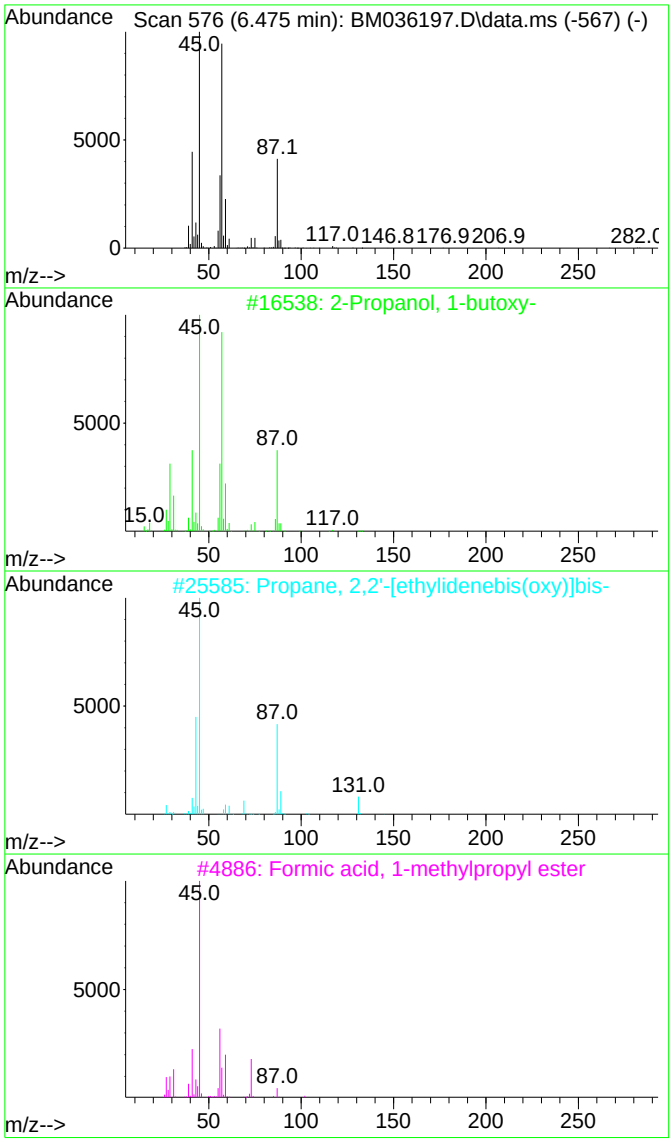
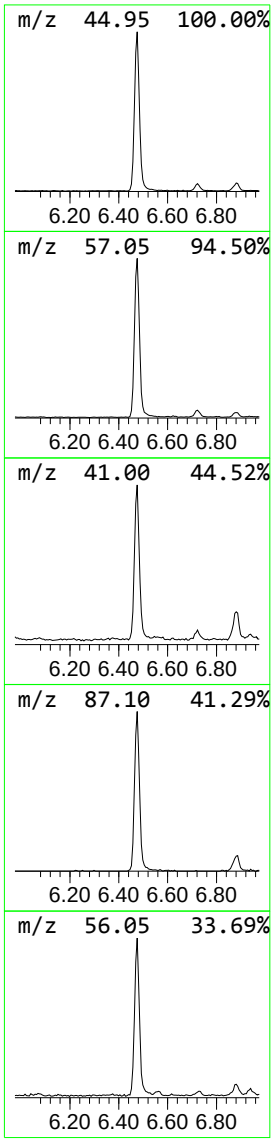
Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.475	7.72 ng	557952	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	Propane, 2,2'-[ethylidenebis(oxy...	146	C8H18O2	004285-59-0	50
3	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	50
4	Propane, 1,1'-[ethylidenebis(oxy...	146	C8H18O2	000105-82-8	50
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	47





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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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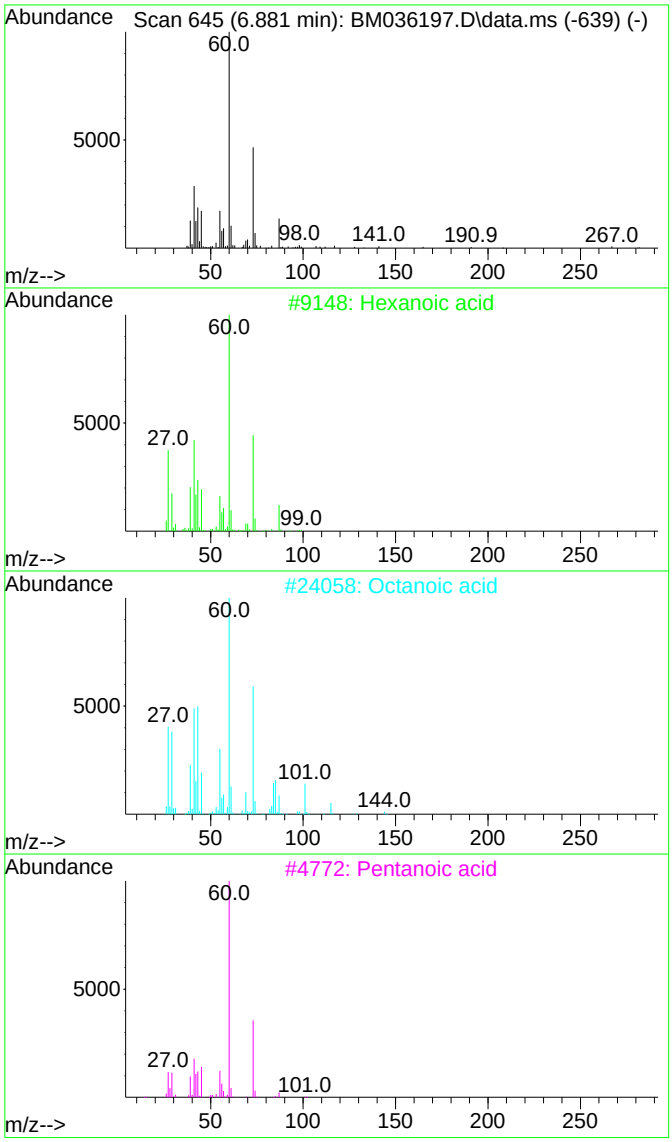
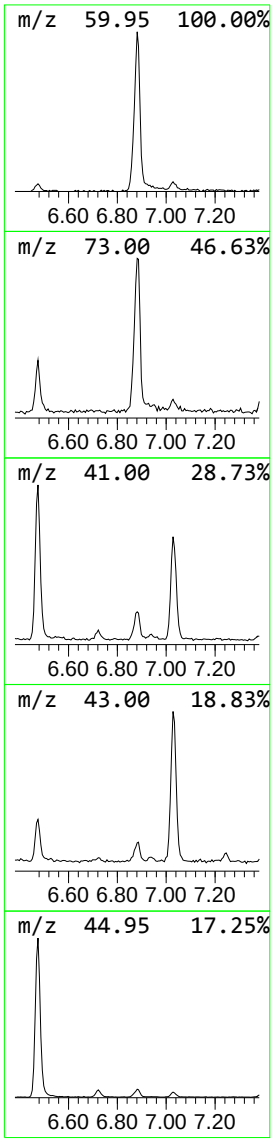
Peak Number 5 Hexanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.881	2.03 ng	146906	1,4-Dichlorobenzene-d4	7.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	83
2	Octanoic acid	144	C8H16O2	000124-07-2	74
3	Pentanoic acid	102	C5H10O2	000109-52-4	72
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
5	Heptanoic acid	130	C7H14O2	000111-14-8	56





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TIC Library : C:\Database\NIST20.L
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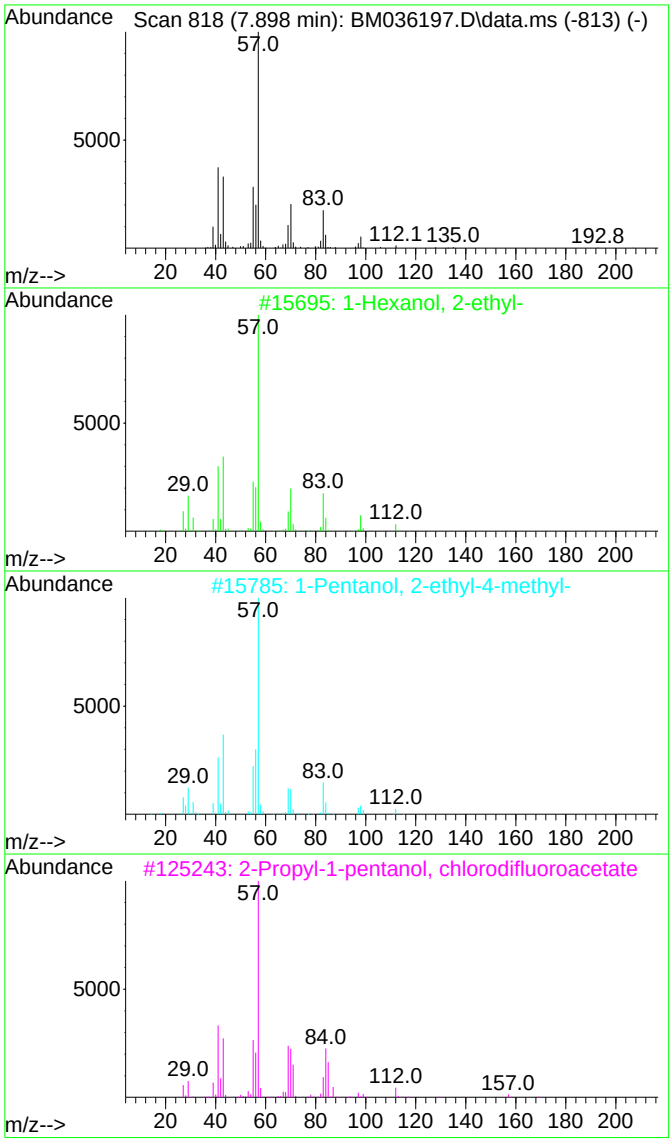
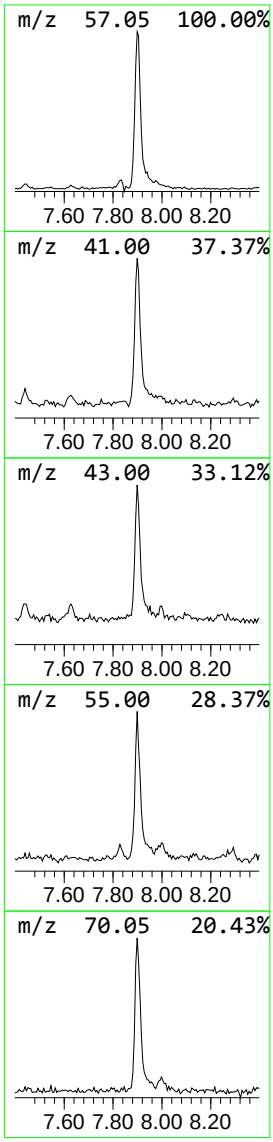
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	2.78 ng	201107	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	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	53
4	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	47
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47





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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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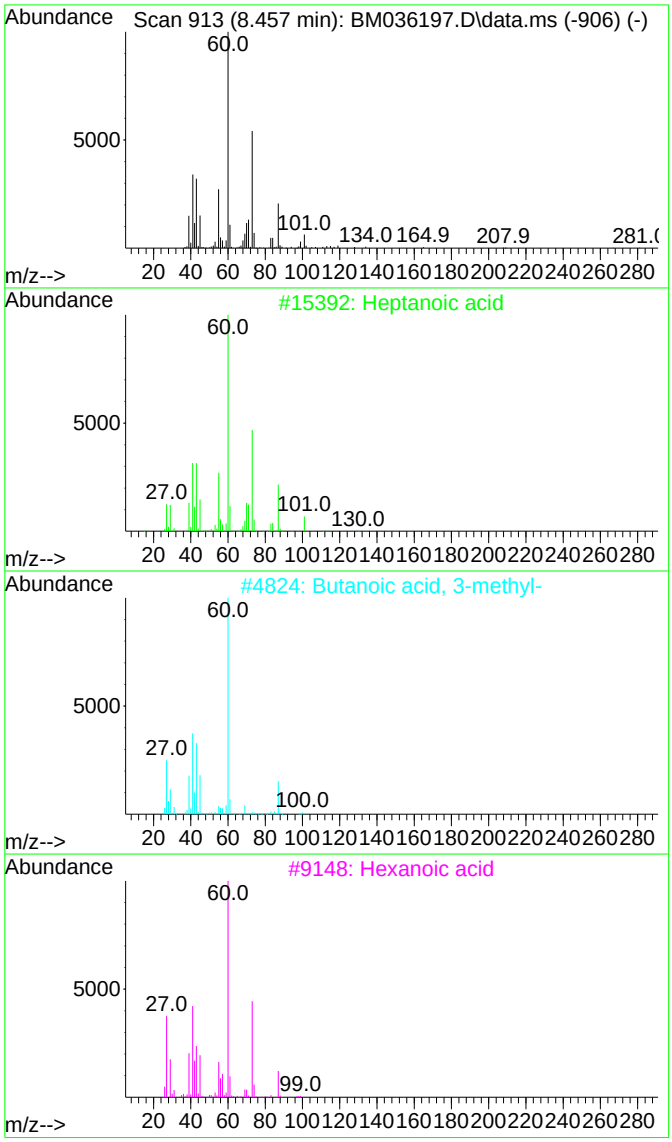
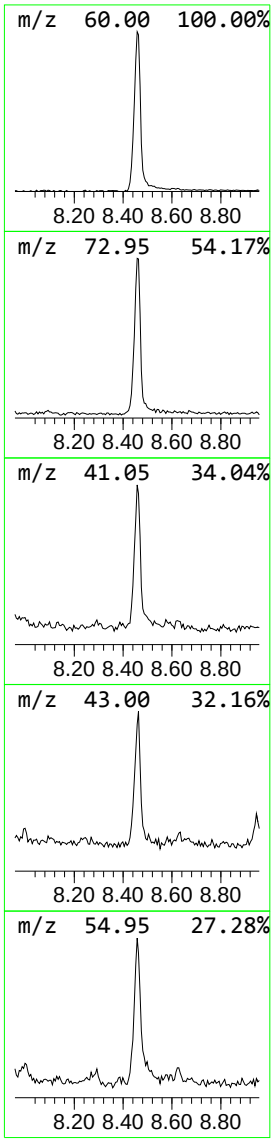
Peak Number 7 Heptanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	3.59 ng	259316	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	59
3	Hexanoic acid	116	C6H12O2	000142-62-1	56
4	Pentanoic acid	102	C5H10O2	000109-52-4	53
5	Octanoic acid	144	C8H16O2	000124-07-2	45





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TIC Library : C:\Database\NIST20.L
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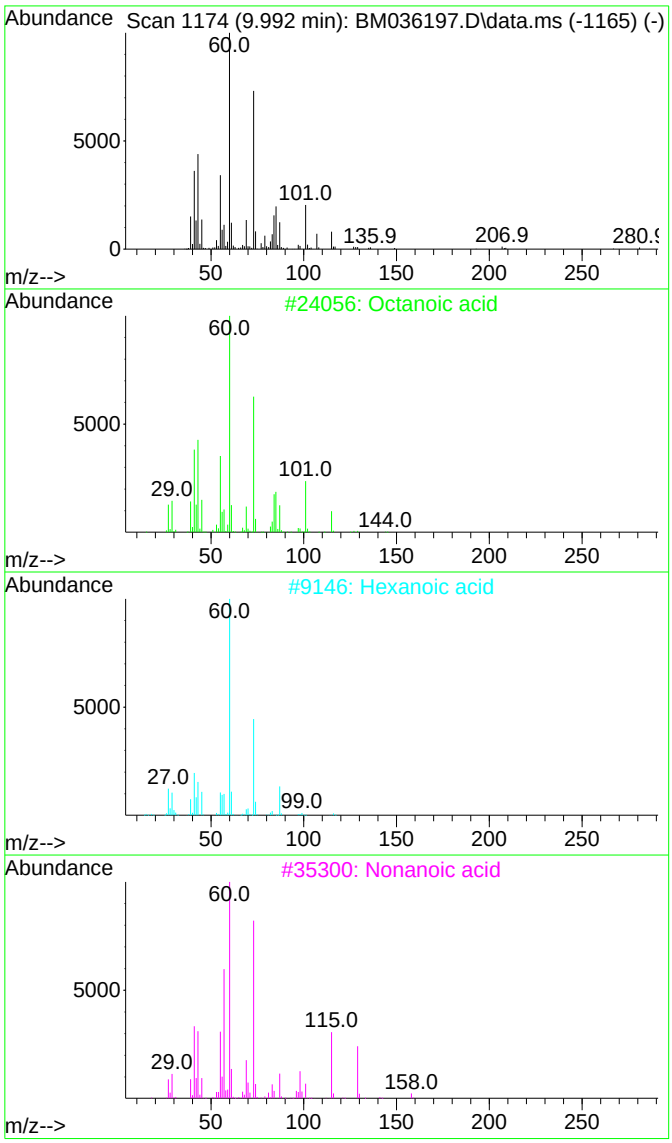
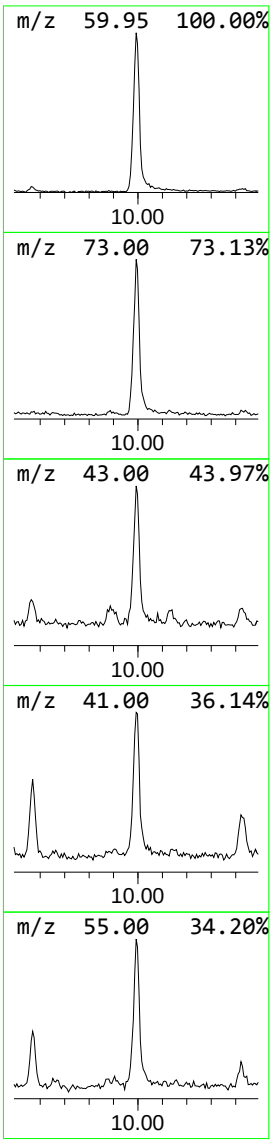
Peak Number 8 Octanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.992	3.09 ng	304077	Naphthalene-d8	10.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	91
2	Hexanoic acid	116	C6H12O2	000142-62-1	60
3	Nonanoic acid	158	C9H18O2	000112-05-0	50
4	Pentanoic acid	102	C5H10O2	000109-52-4	50
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43





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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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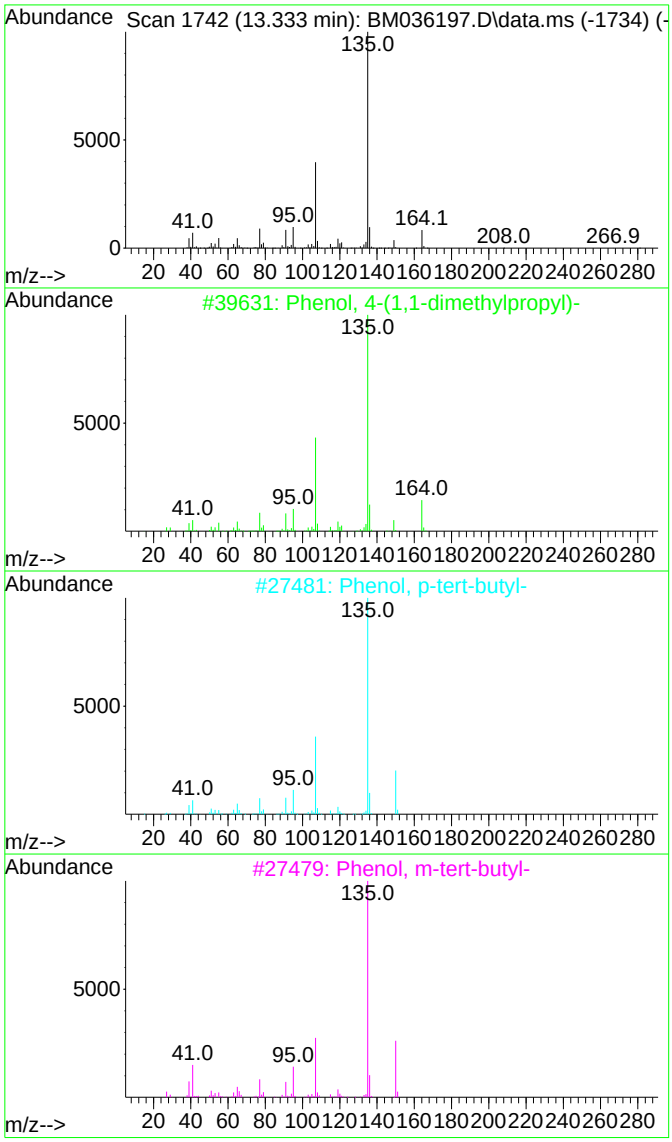
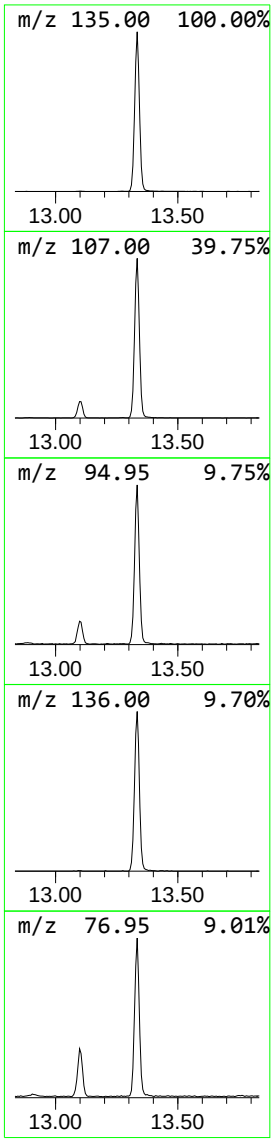
Peak Number 9 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	23.12 ng	2738540	Acenaphthene-d10	14.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	80
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
5	Hexestrol, O-(n-propyloxycarbonyl)-	356	C22H28O4	1000487-65-1	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036197.D
Acq On : 10 Aug 2022 18:09
Operator : CG/JU
Sample : N3972-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-15

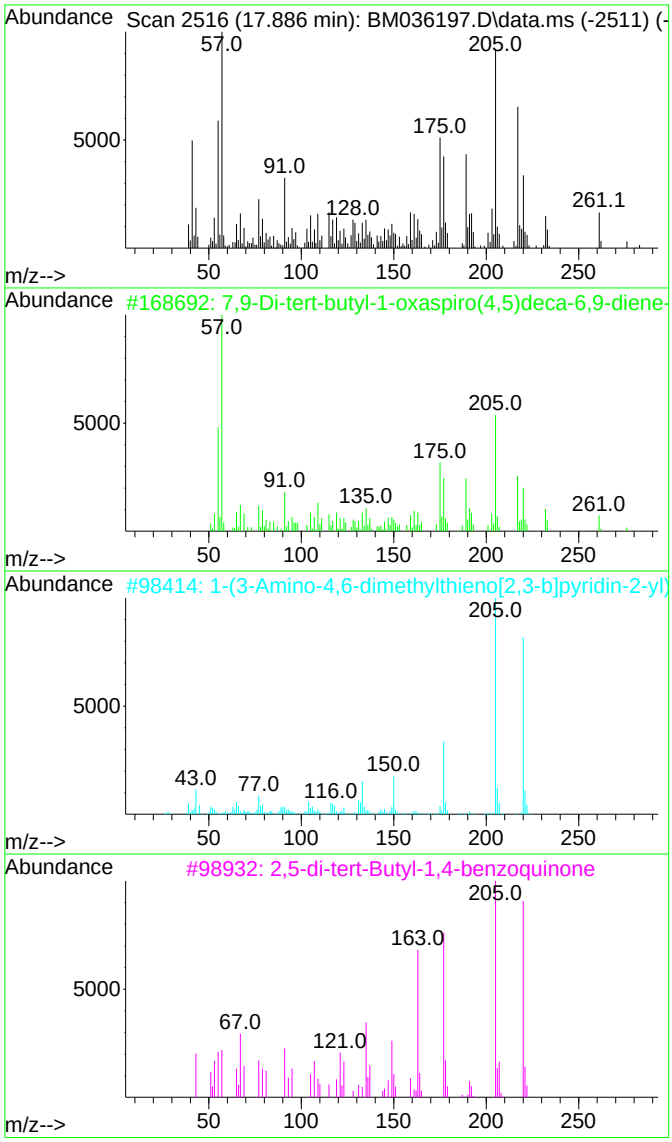
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

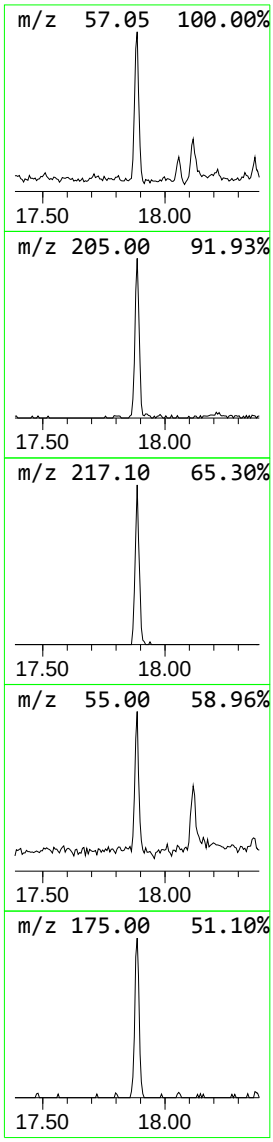
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.886	2.08 ng	266586	Phenanthrene-d10	17.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	50
3	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	46
4	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	38
5	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081022\
Data File : BM036197.D
Acq On : 10 Aug 2022 18:09
Operator : CG/JU
Sample : N3972-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SPN-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	18.9	ng	1362370	1	7.834	1445540	20.0
Ethanol, 2-(1-m...	4.922	7.1	ng	510030	1	7.834	1445540	20.0
1-Hexanol	5.322	2.1	ng	152648	1	7.834	1445540	20.0
2-Propanol, 1-b...	6.475	7.7	ng	557952	1	7.834	1445540	20.0
Hexanoic acid	6.881	2.0	ng	146906	1	7.834	1445540	20.0
1-Hexanol, 2-et...	7.898	2.8	ng	201107	1	7.834	1445540	20.0
Heptanoic acid	8.457	3.6	ng	259316	1	7.834	1445540	20.0
Octanoic acid	9.992	3.1	ng	304077	2	10.634	1966080	20.0
Phenol, 4-(1,1-...	13.333	23.1	ng	2738540	3	14.475	2369300	20.0
7,9-Di-tert-but...	17.886	2.1	ng	266586	4	17.215	2563390	20.0