LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081122\
Data File : BM036214.D
Acq On : 11 Aug 2022 18:08
Operator : CG/JU
Sample : N3972-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2022-07-28

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: BM036214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.275	197	202	213	rBV	1233110	1772204	9.96%	2.440%
2	4.916	305	311	320	rBV2	298990	477386	2.68%	0.657%
3	5.404	388	394	408	rVB	1913564	2807172	15.78%	3.865%
4	6.469	570	575	586	rVB	347873	512614	2.88%	0.706%
5	7.022	662	669	682	rVB	1127556	1802685	10.13%	2.482%
6	7.828	796	806	812	rBV	749494	1213121	6.82%	1.670%
7	8.998	998	1005	1024	rVV	2606615	4205711	23.64%	5.791%
8	9.157	1024	1032	1045	rVB3	89300	238307	1.34%	0.328%
9	9.563	1095	1101	1109	rVB	167208	264759	1.49%	0.365%
10	10.628	1275	1282	1291	rBV	1064762	1775619	9.98%	2.445%
11	11.004	1340	1346	1361	rBV	93848	232367	1.31%	0.320%
12	11.457	1417	1423	1434	rVB2	112821	226729	1.27%	0.312%
13	11.598	1442	1447	1458	rVB2	75630	179260	1.01%	0.247%
14	12.833	1652	1657	1664	rBV	146421	248659	1.40%	0.342%
15	13.098	1692	1702	1715	rBV	6750631	10316196	57.98%	14.204%
16	13.327	1733	1741	1747	rBV	2303769	3267493	18.36%	4.499%
17	14.469	1928	1935	1943	rVB	1789432	2531827	14.23%	3.486%
18	15.292	2068	2075	2081	rVB	161930	245281	1.38%	0.338%
19	15.827	2161	2166	2171	rBV	192346	264534	1.49%	0.364%
20	15.963	2181	2189	2205	rBV	6217741	8925443	50.16%	12.289%
21	16.557	2283	2290	2298	rBV2	146909	272813	1.53%	0.376%
22	17.210	2395	2401	2409	rBV	2293159	3215093	18.07%	4.427%
23	17.880	2510	2515	2521	rVB	294499	361897	2.03%	0.498%
24	18.110	2549	2554	2560	rBV	123657	188463	1.06%	0.259%
25	18.186	2562	2567	2575	rVB	176810	266242	1.50%	0.367%
26	19.839	2842	2848	2855	rBV	14473715	17792799	100.00%	24.498%
27	20.603	2974	2978	2982	rBV	345343	390282	2.19%	0.537%
28	21.392	3108	3112	3118	rBV	3193553	3937626	22.13%	5.421%
29	22.480	3294	3297	3308	rVB	399111	552940	3.11%	0.761%
30	23.739	3505	3511	3523	rVB2	2107258	4144307	23.29%	5.706%

Sum of corrected areas: 72629829

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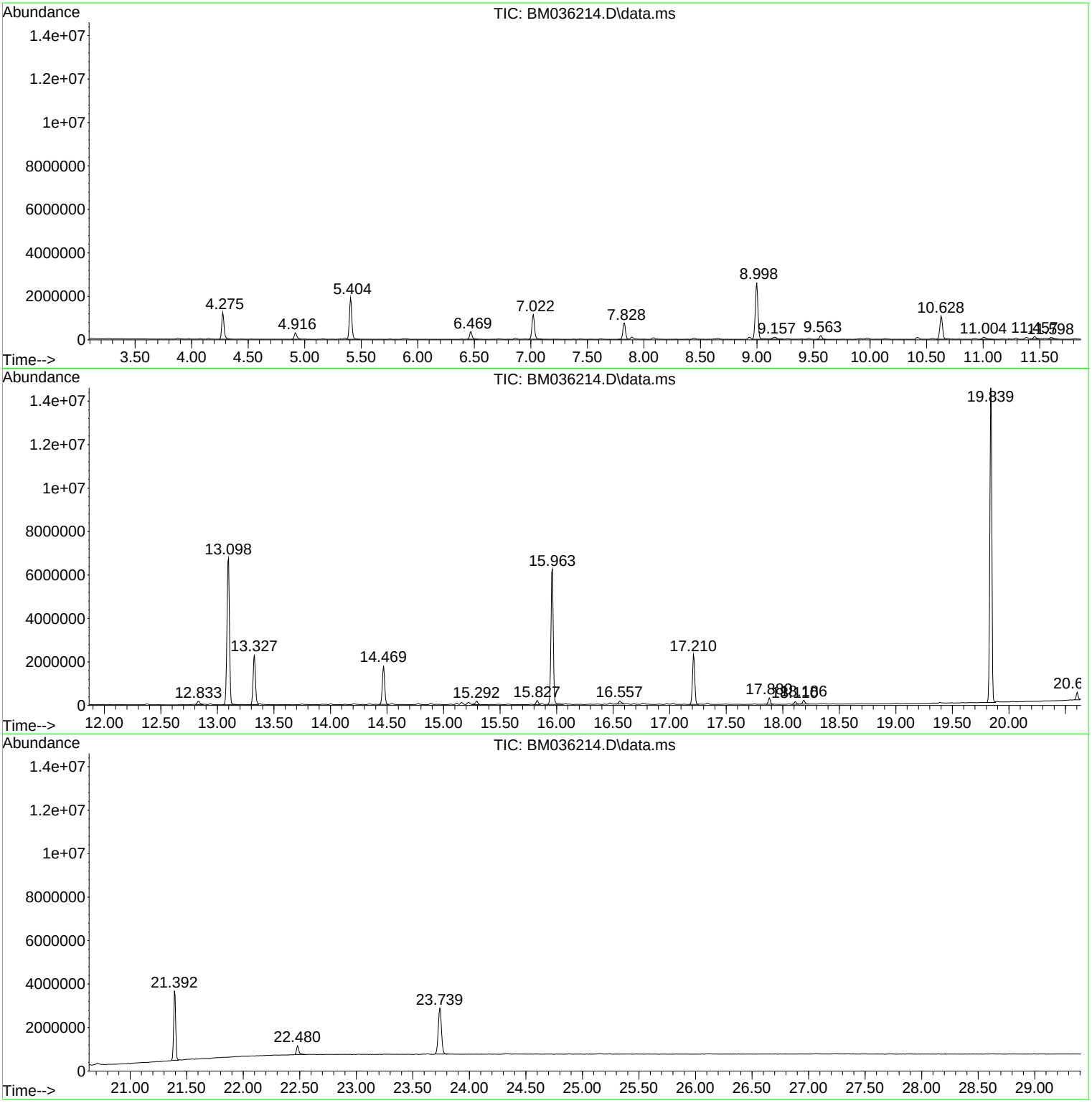
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2022-07-28

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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TIC Library : C:\Database\NIST20.L
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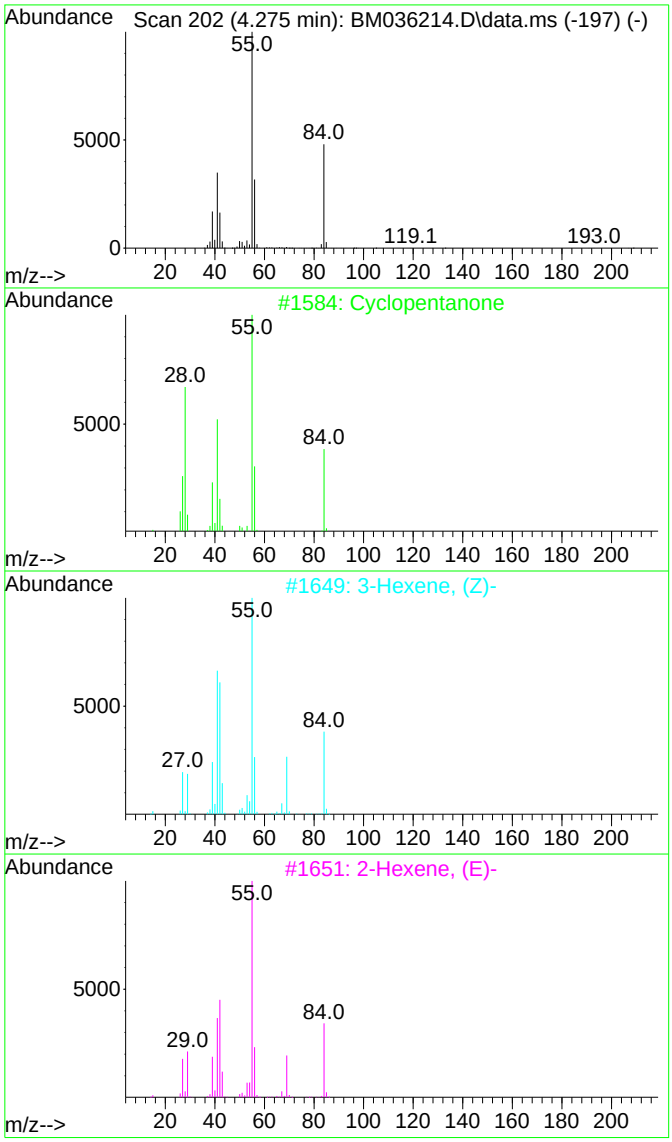
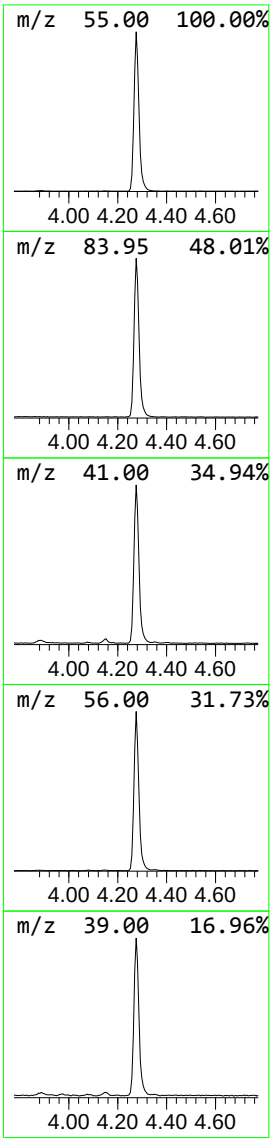
****

Peak Number 1 Cyclopentanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.275	29.22 ng	1772200	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	3-Hexene, (Z)-	84	C6H12	007642-09-3	59
3	2-Hexene, (E)-	84	C6H12	004050-45-7	59
4	2(5H)-Furanone	84	C4H4O2	000497-23-4	52
5	2(3H)-Furanone	84	C4H4O2	020825-71-2	38





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Sample : N3972-09
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Instrument :
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ClientSampleId :
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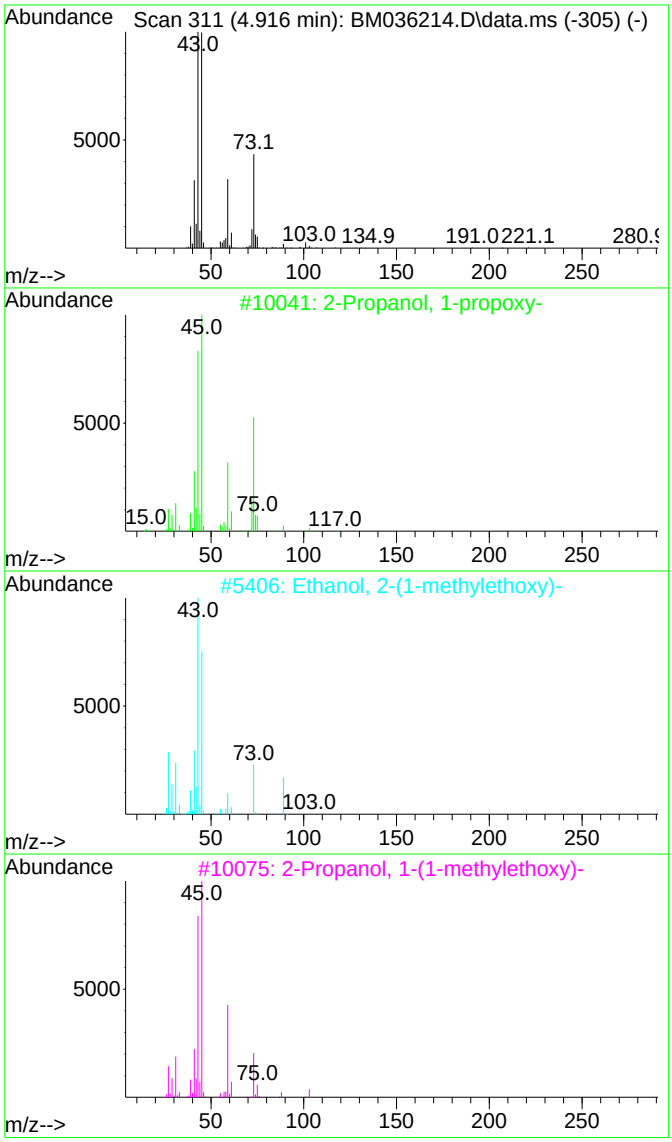
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

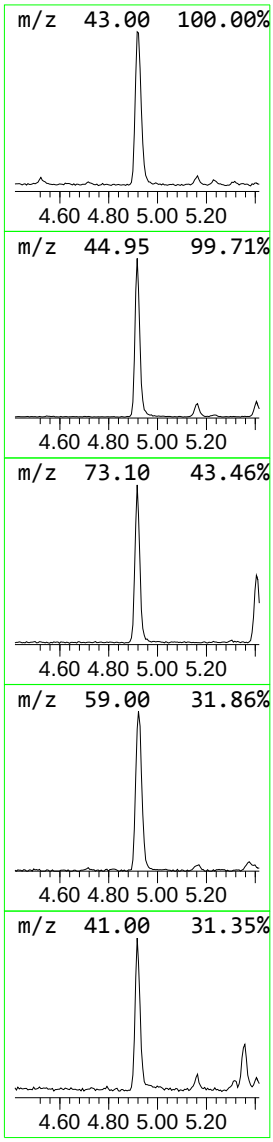
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanol, 1-propoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.916	7.87 ng	477386	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	78
2	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	78
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
4	Sulfurous acid, bis(1-methylethy...	166	C6H14O3S	004773-13-1	50
5	Methoxyacetic acid, hexyl ester	174	C9H18O3	145747-16-6	45





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Sample : N3972-09
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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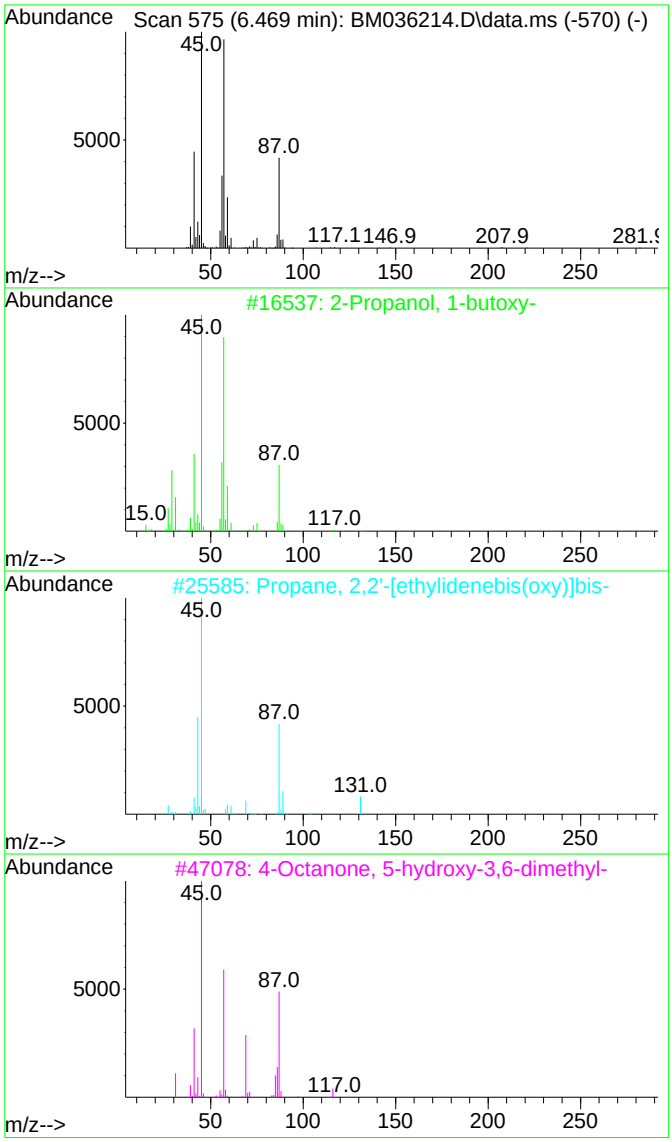
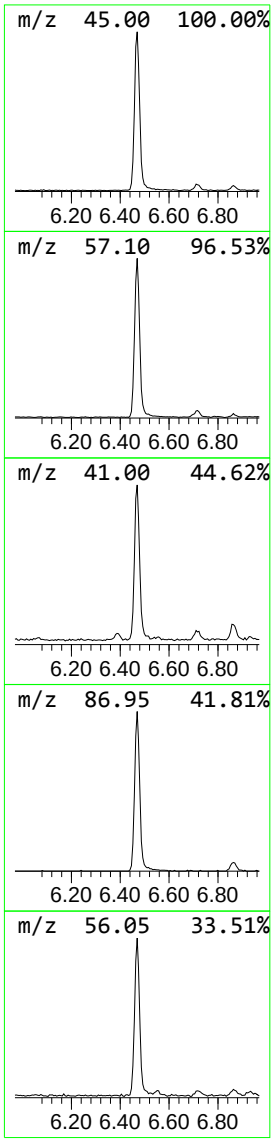
Peak Number 3 2-Propanol, 1-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.469	8.45 ng	512614	1,4-Dichlorobenzene-d4	7.828

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	4-Octanone, 5-hydroxy-3,6-dimethyl-	172	C10H20O2	062759-47-1	42
4	Diisopropyl ether	102	C6H14O	000108-20-3	42
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42





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Acq On : 11 Aug 2022 18:08
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Sample : N3972-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

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

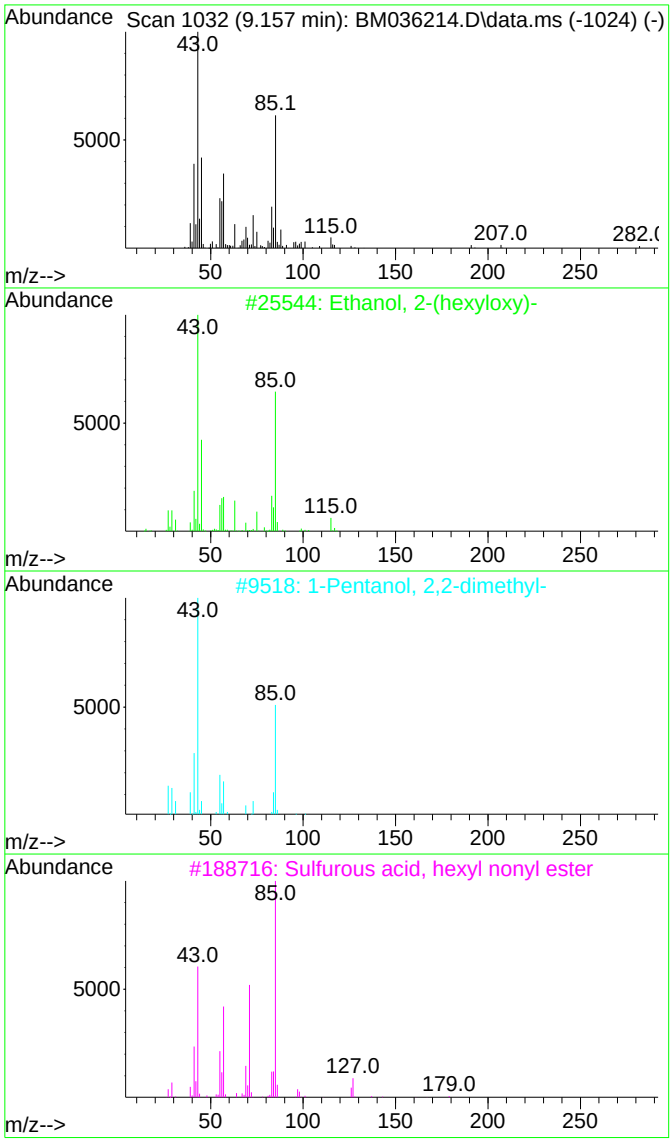
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

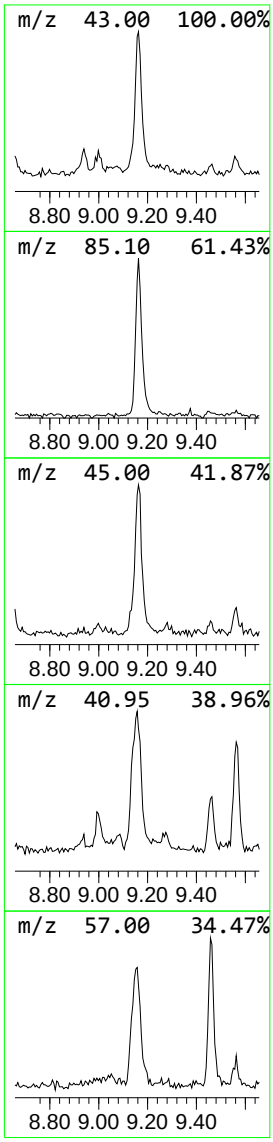
****

Peak Number 4 Ethanol, 2-(hexyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	3.93 ng	238307	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexyloxy)-	146	C8H18O2	000112-25-4	53
2	1-Pentanol, 2,2-dimethyl-	116	C7H16O	002370-12-9	38
3	Sulfurous acid, hexyl nonyl ester	292	C15H32O3S	1000309-13-1	35
4	Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	35
5	Nonane, 5-methyl-	142	C10H22	015869-85-9	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081122\
Data File : BM036214.D
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Operator : CG/JU
Sample : N3972-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2022-07-28

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
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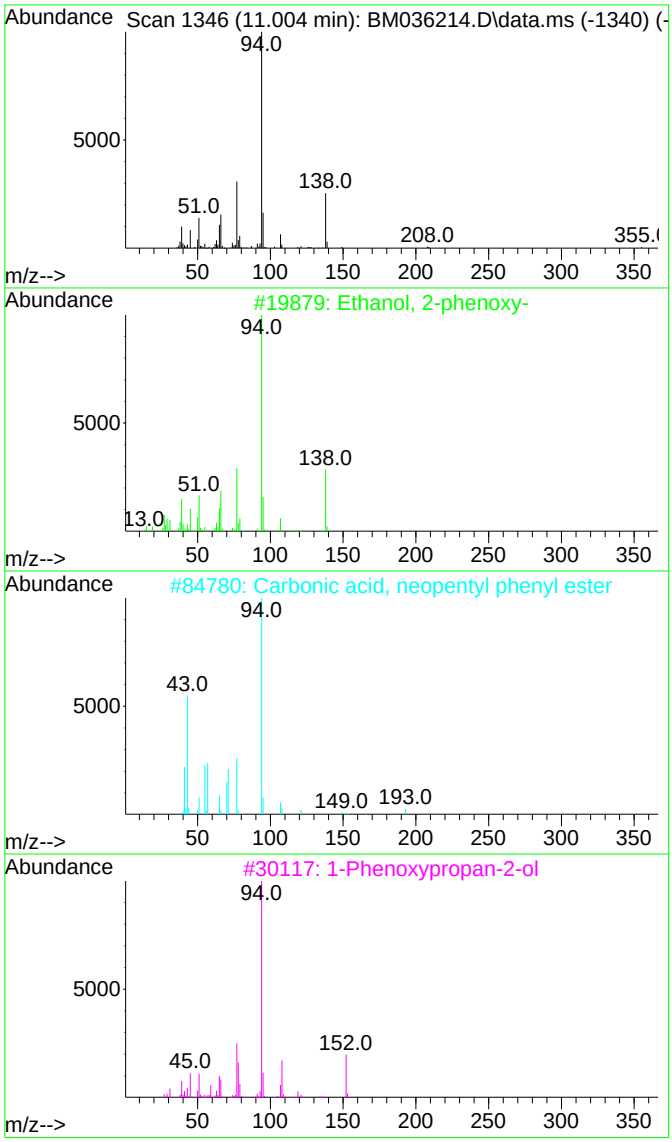
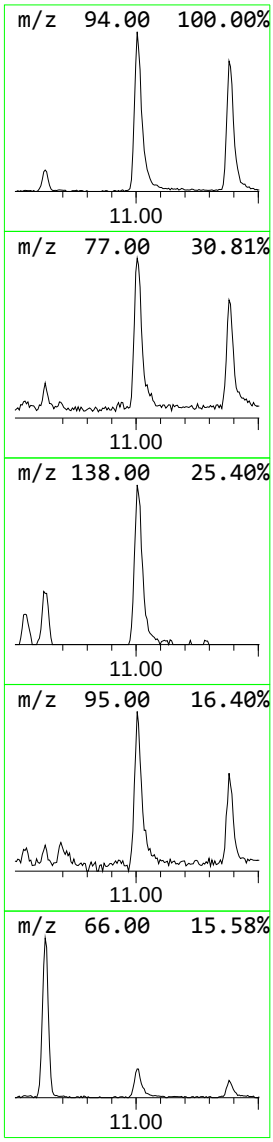
****

Peak Number 5 Ethanol, 2-phenoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.004	2.62 ng	232367	Naphthalene-d8	10.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	96
2	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	72
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	64
4	2-Phenoxybutyric acid	180	C10H12O3	013794-14-4	59
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	59





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TIC Library : C:\Database\NIST20.L
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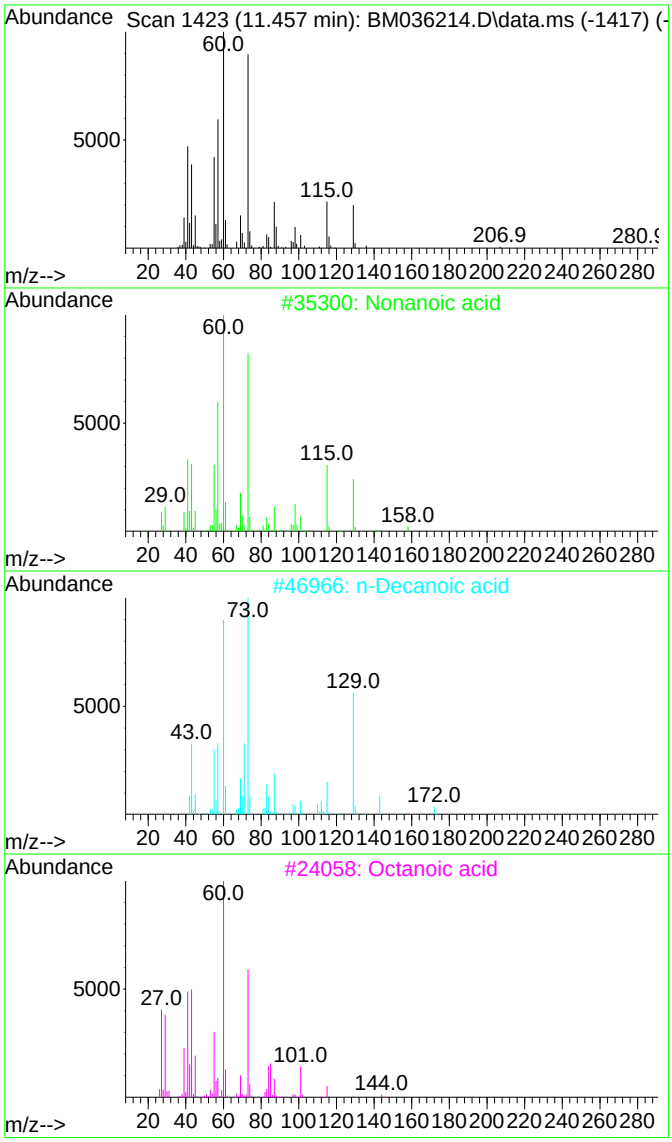
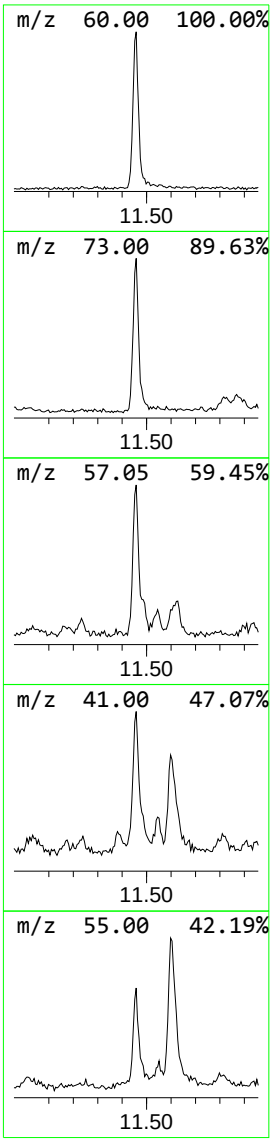
****

Peak Number 6 Nonanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.457	2.55 ng	226729	Naphthalene-d8	10.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	45
3	Octanoic acid	144	C8H16O2	000124-07-2	43
4	Hexanoic acid	116	C6H12O2	000142-62-1	43
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43





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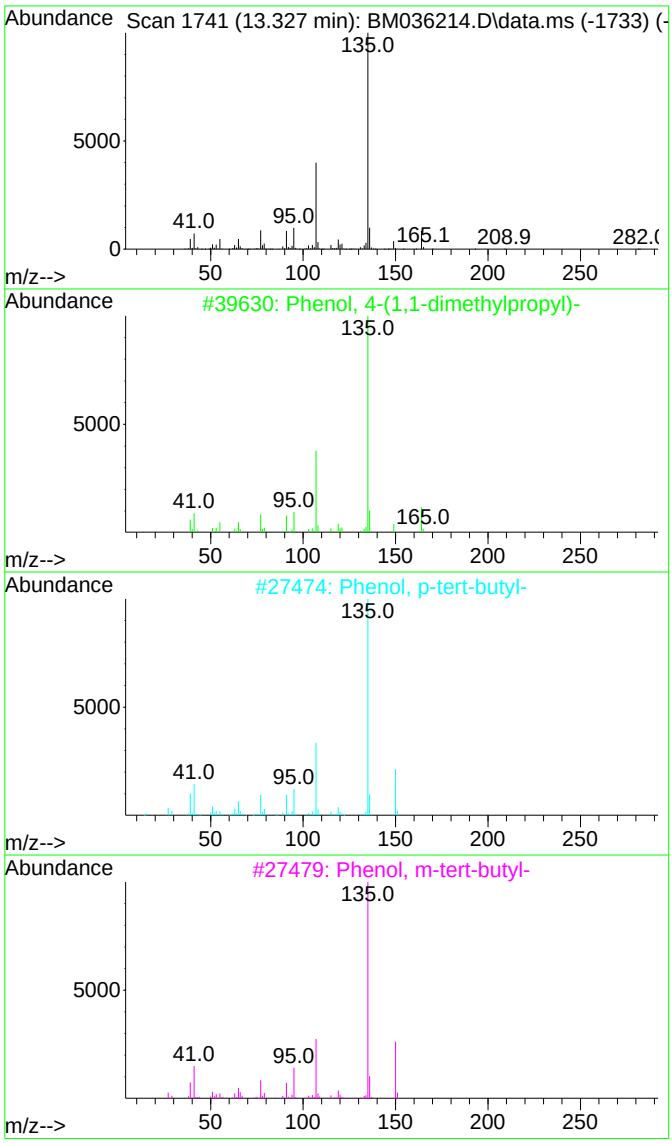
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

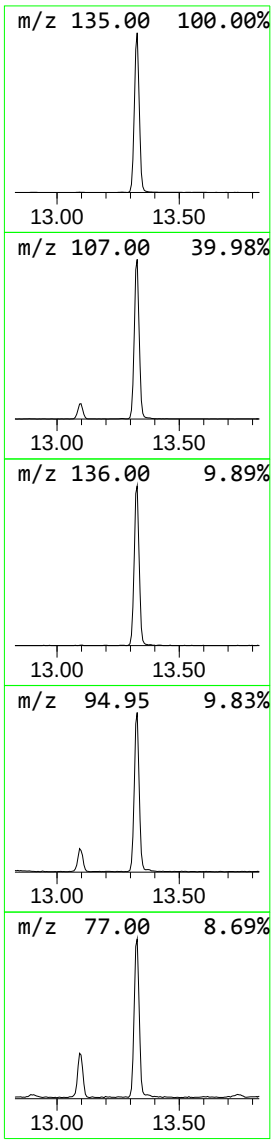
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.328	25.81 ng	3267490	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	86
4	4,6-Bis(4-ethoxybenzylthio)-5-ni...	457	C22H23N3O4S2	325957-76-4	64
5	Hexestrol, O-isopropyloxycarbonyl-	356	C22H28O4	1000487-68-4	64





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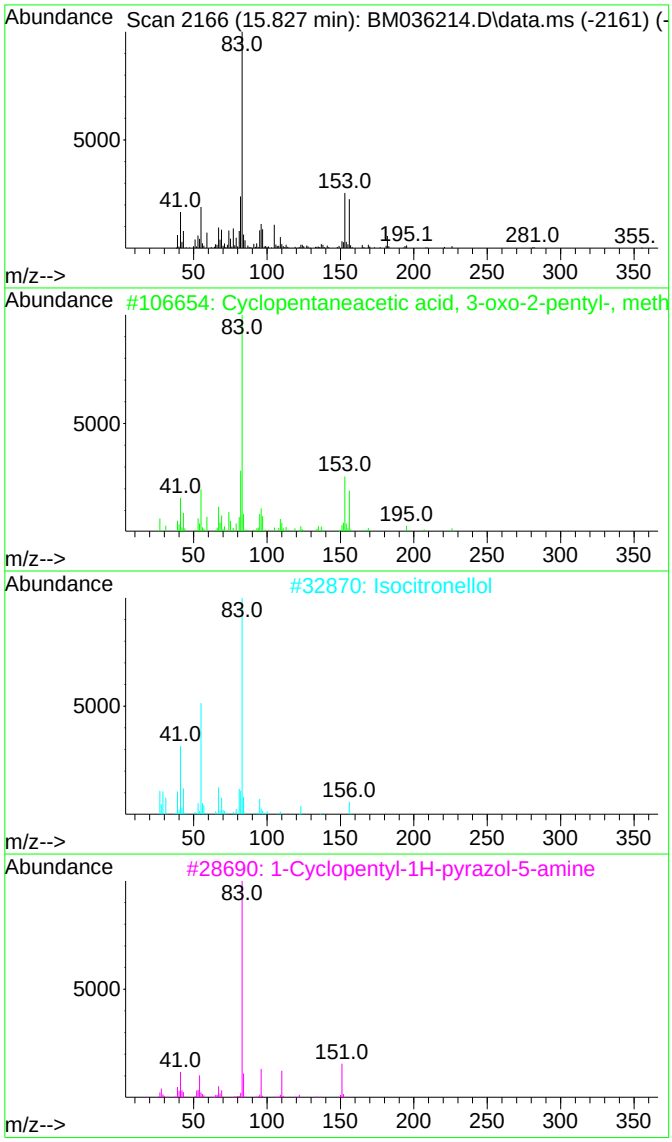
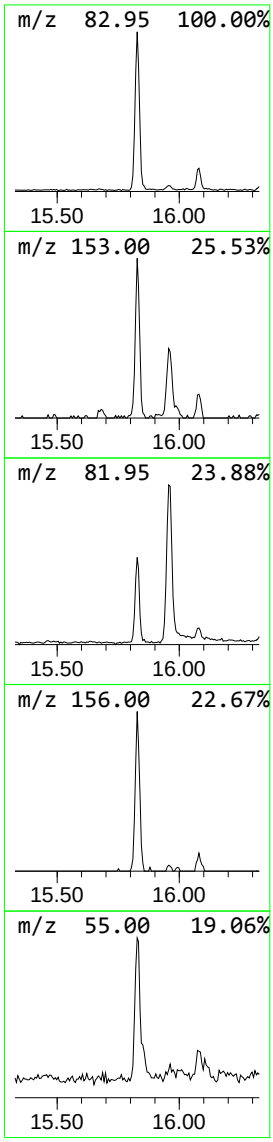
****
Peak Number 8 Cyclopentaneacetic acid, 3-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	2.09 ng	264534	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	87
2	Isocitronellol	156	C10H20O	018479-52-2	50
3	1-Cyclopentyl-1H-pyrazol-5-amine	151	C8H13N3	003702-09-8	43
4	Cyclohexane, 1,1'-(1,5-pentanedi...	236	C17H32	054833-31-7	38
5	Phomopsolide B, diacetate	380	C19H24O8	097533-95-4	38





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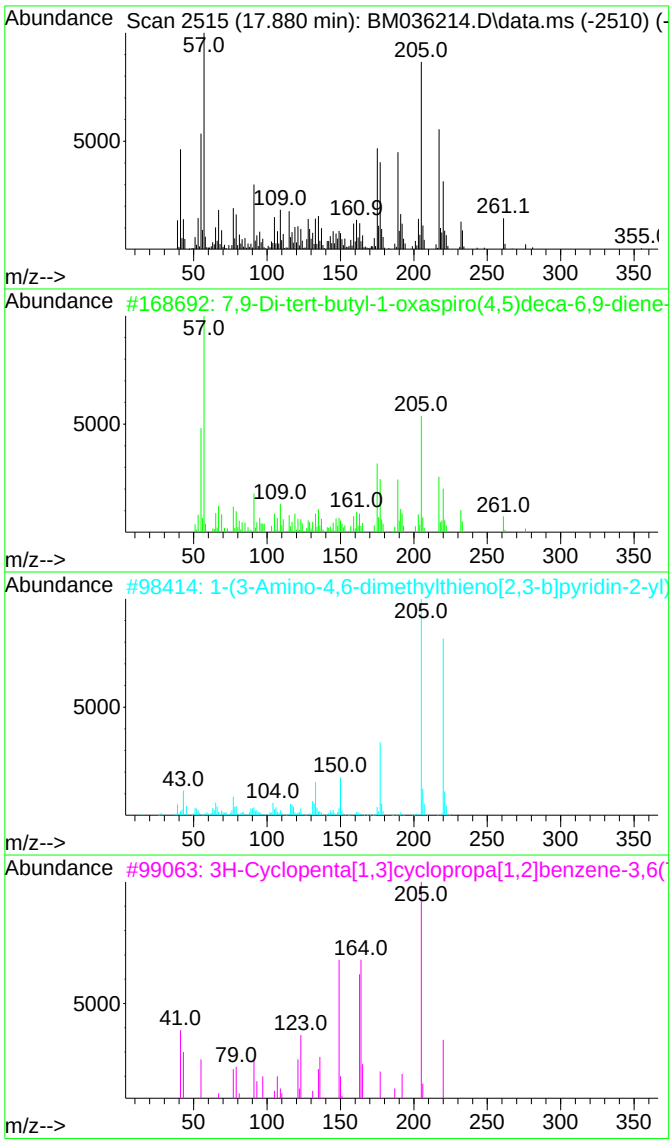
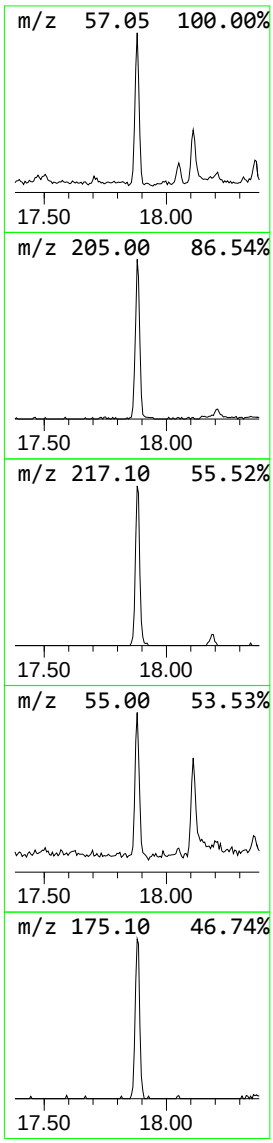
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.880	2.25 ng	361897	Phenanthrene-d10	17.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45
3	3H-Cyclopenta[1,3]cyclopropa[1,2...	220	C14H20O2	066708-18-7	38
4	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	38
5	Ethyl 4-acetyl-3,5-dimethylbenzoate	220	C13H16O3	1000431-98-6	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081122\
Data File : BM036214.D
Acq On : 11 Aug 2022 18:08
Operator : CG/JU
Sample : N3972-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2022-07-28

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

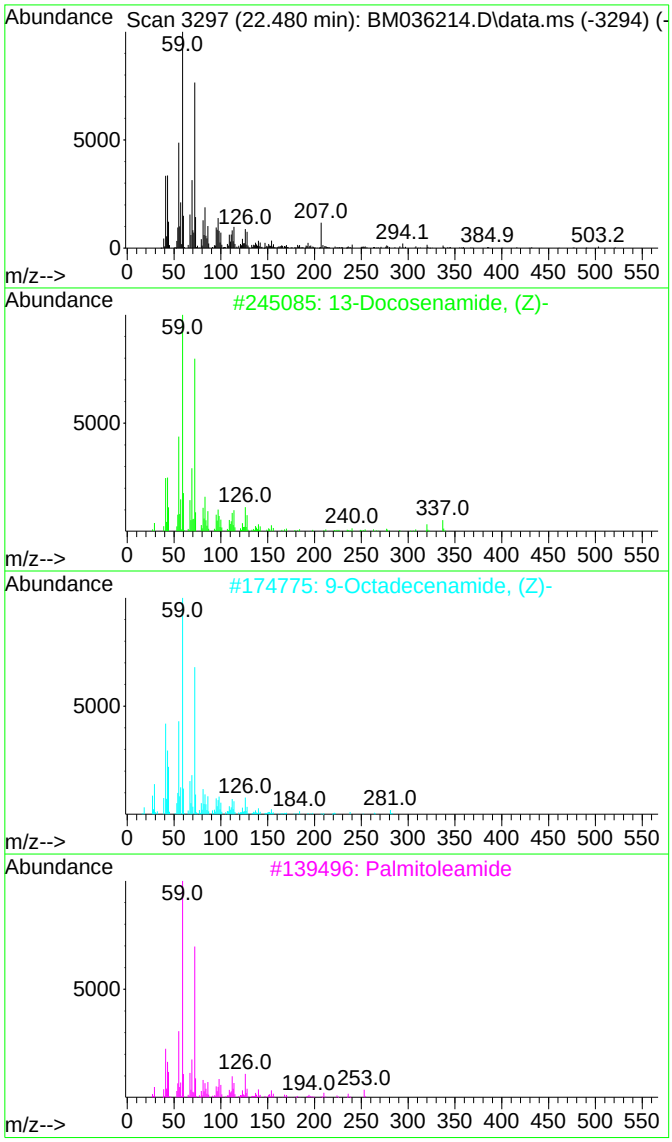
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

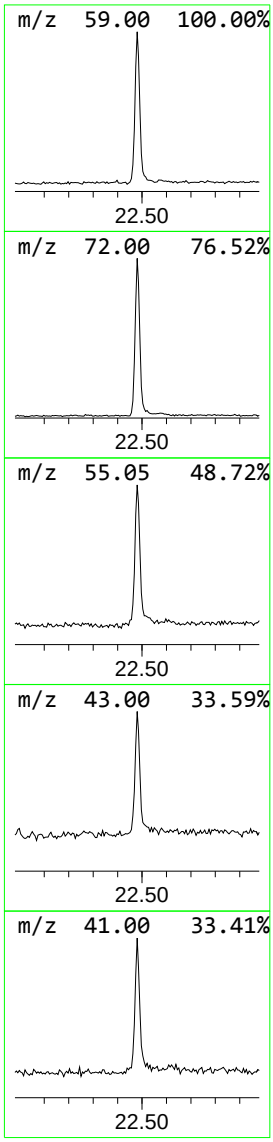
****

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.480	2.81 ng	552940	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	Palmitoleamide	253	C16H31NO	106010-22-4	64
4	Octadecanamide	283	C18H37NO	000124-26-5	50
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081122\
Data File : BM036214.D
Acq On : 11 Aug 2022 18:08
Operator : CG/JU
Sample : N3972-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2022-07-28

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	4.275	29.2	ng	1772200	1	7.828	1213120	20.0
2-Propanol, 1-p...	4.916	7.9	ng	477386	1	7.828	1213120	20.0
2-Propanol, 1-b...	6.469	8.4	ng	512614	1	7.828	1213120	20.0
Ethanol, 2-(hex...	9.157	3.9	ng	238307	1	7.828	1213120	20.0
Ethanol, 2-phen...	11.004	2.6	ng	232367	2	10.628	1775620	20.0
Nonanoic acid	11.457	2.5	ng	226729	2	10.628	1775620	20.0
Phenol, 4-(1,1-...	13.328	25.8	ng	3267490	3	14.469	2531830	20.0
Cyclopentaneace...	15.827	2.1	ng	264534	3	14.469	2531830	20.0
7,9-Di-tert-but...	17.880	2.3	ng	361897	4	17.210	3215090	20.0
13-Docosenamide...	22.480	2.8	ng	552940	5	21.392	3937630	20.0