LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139309.D
Acq On : 10 Sep 2024 20:00
Operator : RC/JU
Sample : P3853-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
252805

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_F\Methods\8270-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139309.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	10	19	25	rVB	4115559	6885271	100.00%	20.455%
2	5.104	496	512	519	rBV2	90408	187764	2.73%	0.558%
3	5.504	572	580	585	rBV	1138589	1506367	21.88%	4.475%
4	5.645	585	604	608	rVV	86126	271711	3.95%	0.807%
5	5.834	629	636	644	rBV	468669	612472	8.90%	1.820%
6	6.504	743	750	762	rBV	790126	1071003	15.55%	3.182%
7	6.887	810	815	820	rBV	574678	698329	10.14%	2.075%
8	6.945	821	825	832	rVB	148303	189344	2.75%	0.563%
9	7.028	833	839	844	rBV	516514	667536	9.70%	1.983%
10	7.451	903	911	916	rVB	1400781	1916169	27.83%	5.693%
11	7.557	919	929	938	rBV2	49759	146642	2.13%	0.436%
12	7.734	943	959	969	rVB	463279	1327235	19.28%	3.943%
13	8.028	977	1009	1015	rBV	880058	4604970	66.88%	13.681%
14	8.169	1028	1033	1038	rVB	707203	856956	12.45%	2.546%
15	8.481	1083	1086	1091	rVB	59771	79080	1.15%	0.235%
16	8.610	1102	1108	1116	rVB	321592	550846	8.00%	1.636%
17	9.122	1191	1195	1207	rVB	81954	138954	2.02%	0.413%
18	9.245	1210	1216	1221	rBV	2751366	3438273	49.94%	10.215%
19	9.598	1270	1276	1286	rBV	137502	292914	4.25%	0.870%
20	9.922	1326	1331	1336	rVB	713217	881801	12.81%	2.620%
21	10.327	1396	1400	1407	rVB	100316	126280	1.83%	0.375%
22	10.557	1434	1439	1444	rBV	67292	86964	1.26%	0.258%
23	10.710	1460	1465	1470	rBV	1383409	1771796	25.73%	5.264%
24	10.875	1489	1493	1501	rBV	127114	189450	2.75%	0.563%
25	11.127	1531	1536	1544	rVB	237157	299575	4.35%	0.890%
26	11.410	1579	1584	1589	rBV	577984	723123	10.50%	2.148%
27	11.933	1669	1673	1676	rBV	81862	106119	1.54%	0.315%
28	12.657	1794	1796	1803	rVB3	48416	77143	1.12%	0.229%
29	12.851	1825	1829	1842	rBV2	174037	365186	5.30%	1.085%
30	12.998	1848	1854	1859	rBV	1761155	2334104	33.90%	6.934%
31	14.045	2029	2032	2037	rVB	420718	571544	8.30%	1.698%
32	15.527	2281	2284	2308	rVB	280513	685236	9.95%	2.036%

Sum of corrected areas: 33660157

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Misc :
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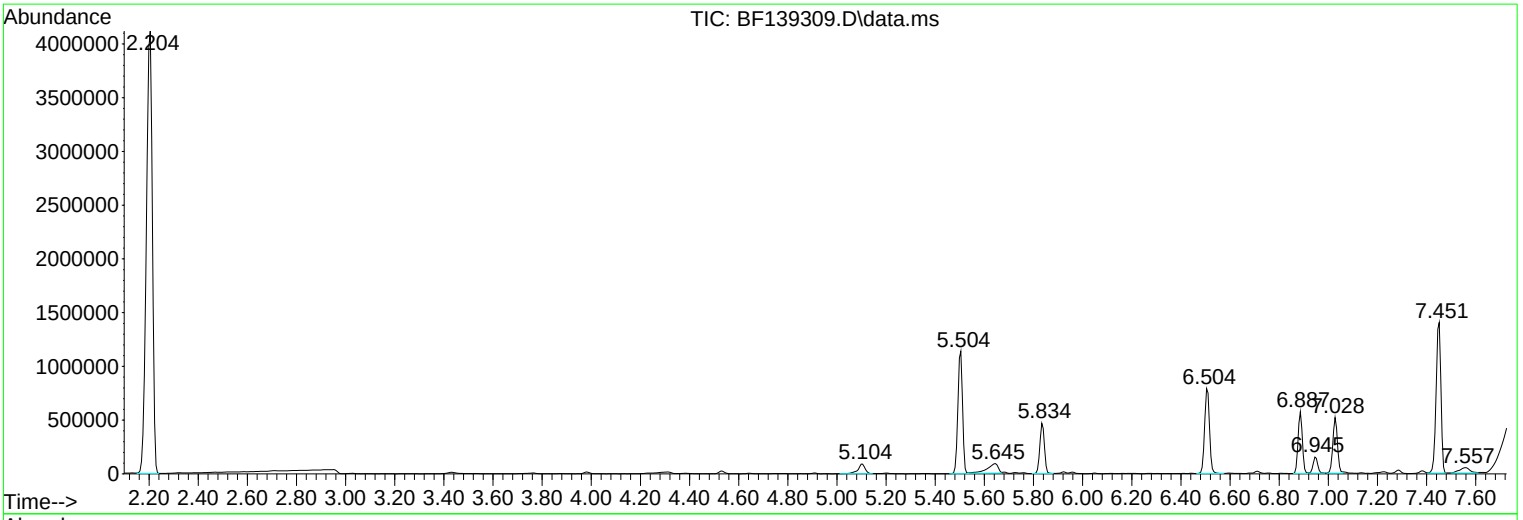
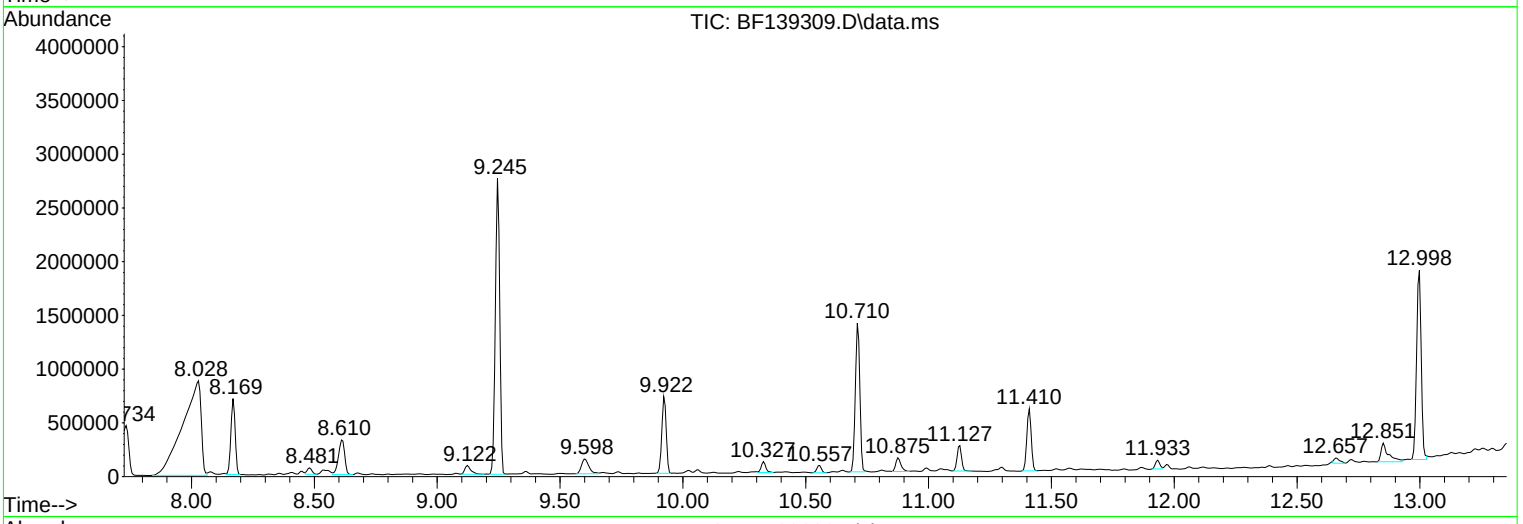
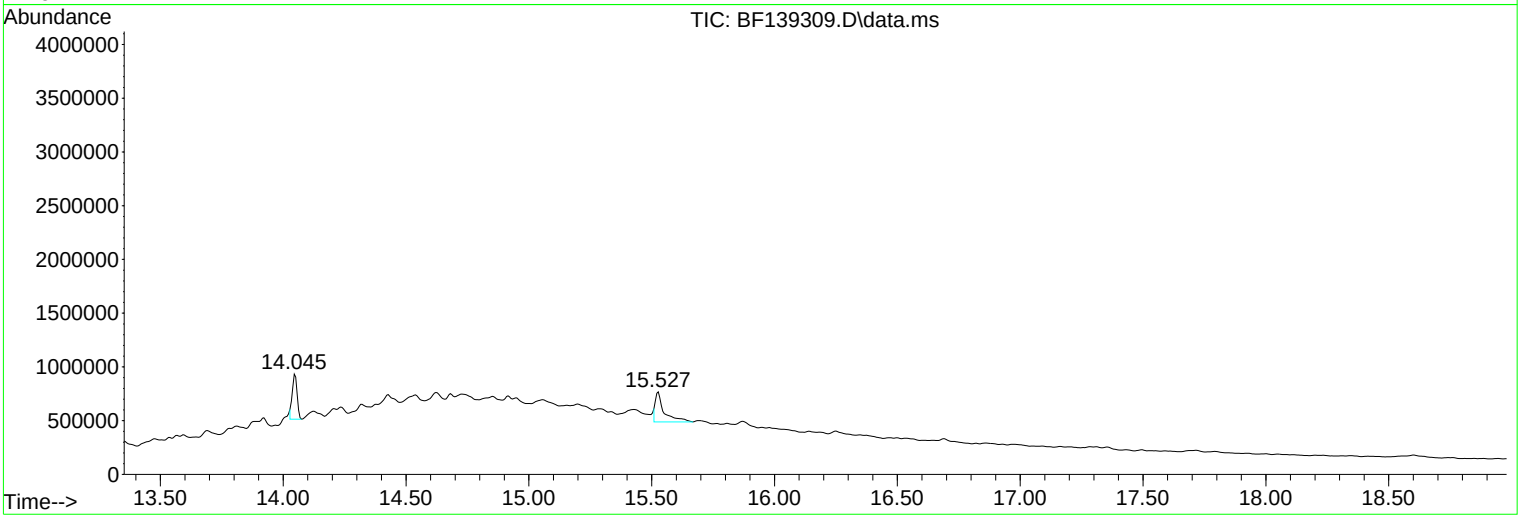
Instrument :
BNA_F
ClientSampleId :
252805

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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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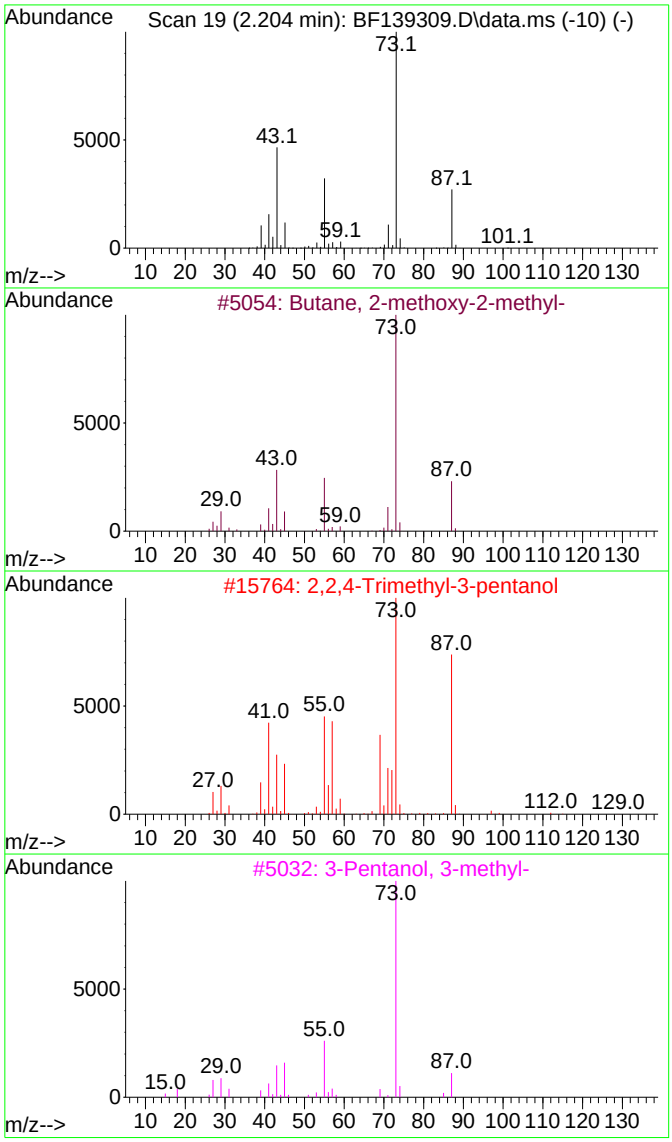
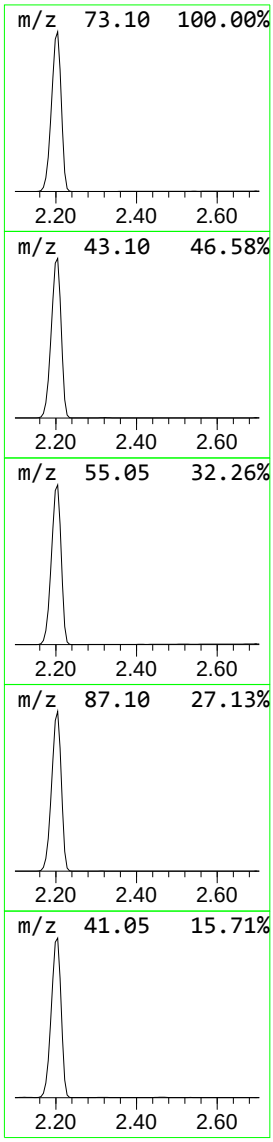
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	197.19 ng	6885270	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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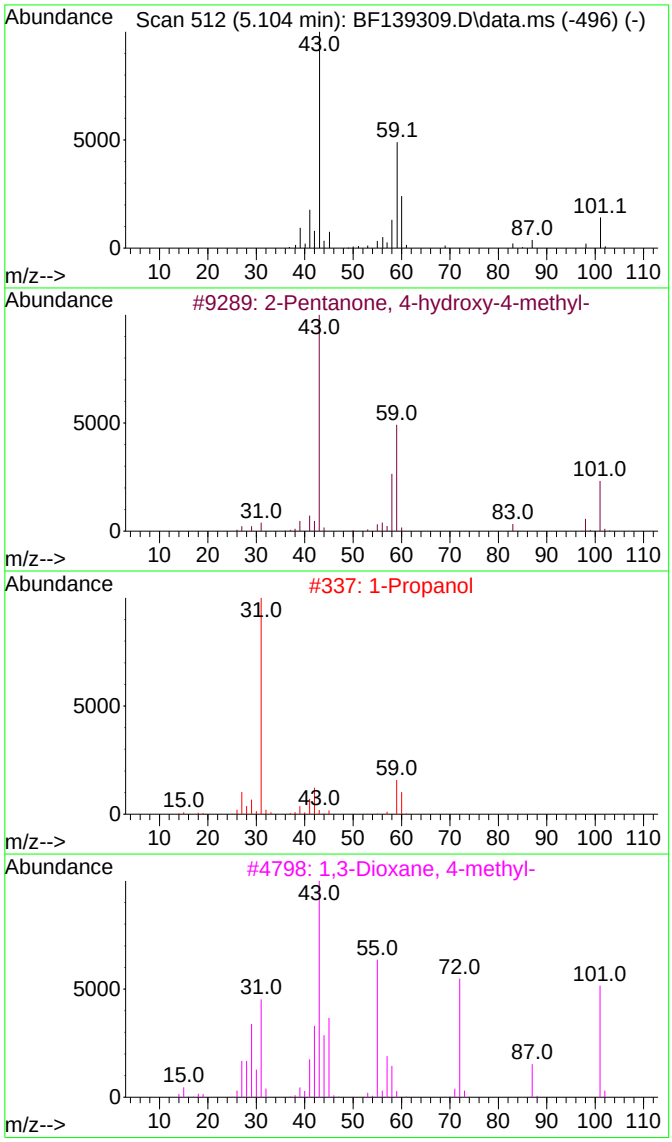
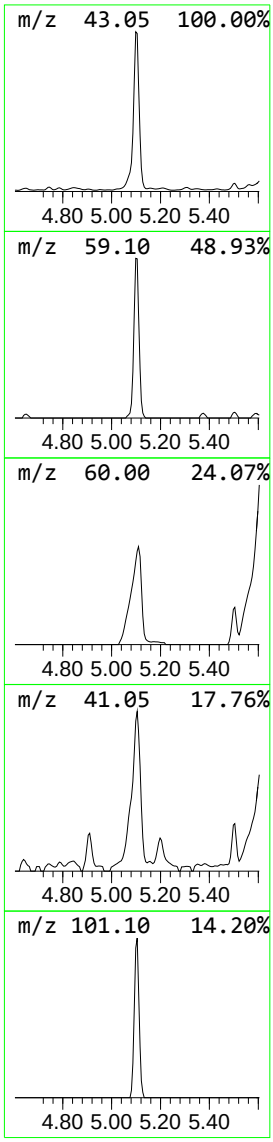
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.38 ng	187764	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	1-Propanol	60	C3H8O	000071-23-8	37
3	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9
4	Propylamine	59	C3H9N	000107-10-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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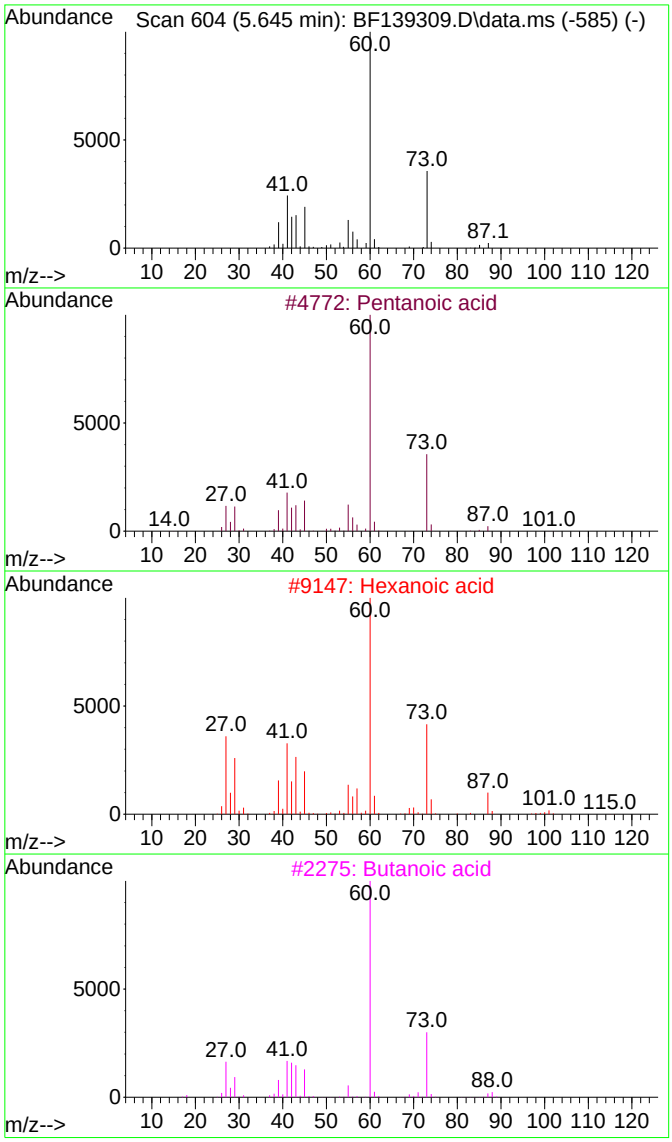
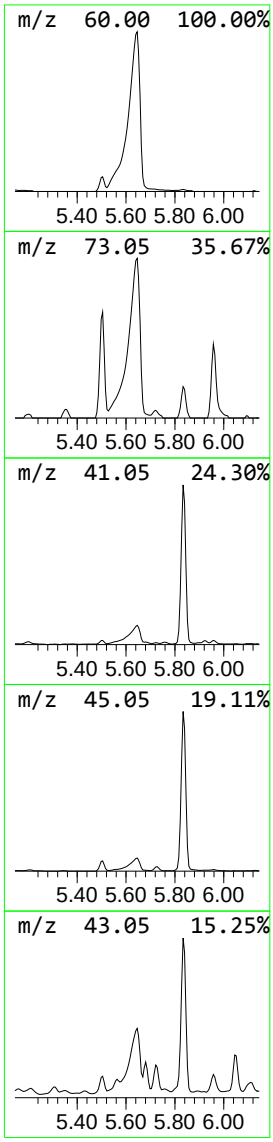
****

Peak Number 3 Pentanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.645	7.78 ng	271711	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	90
2	Hexanoic acid	116	C6H12O2	000142-62-1	64
3	Butanoic acid	88	C4H8O2	000107-92-6	64
4	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	40
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	38





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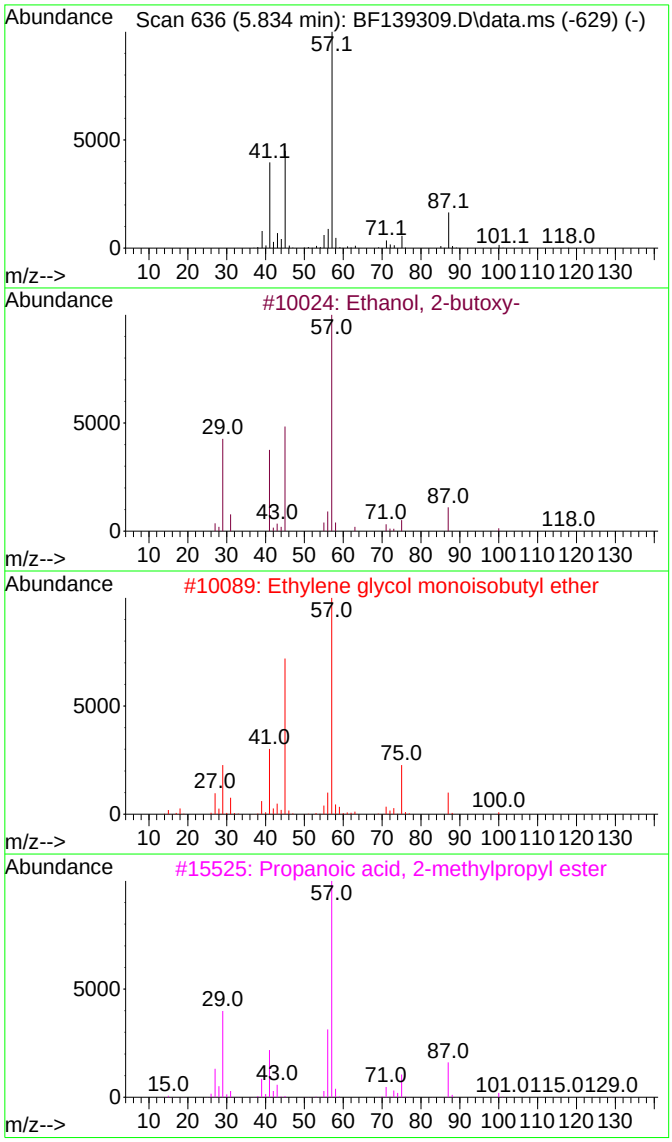
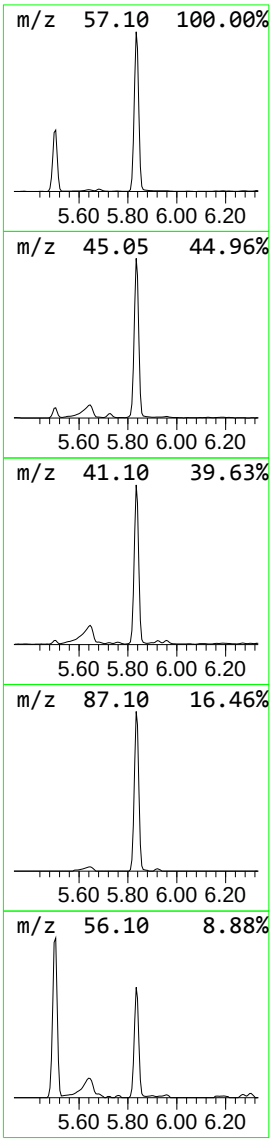
****

Peak Number 4 Ethanol, 2-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	17.54 ng	612472	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
3	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	17
4	1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	17
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	16





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Instrument :
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TIC Library : C:\Database\NIST20.L
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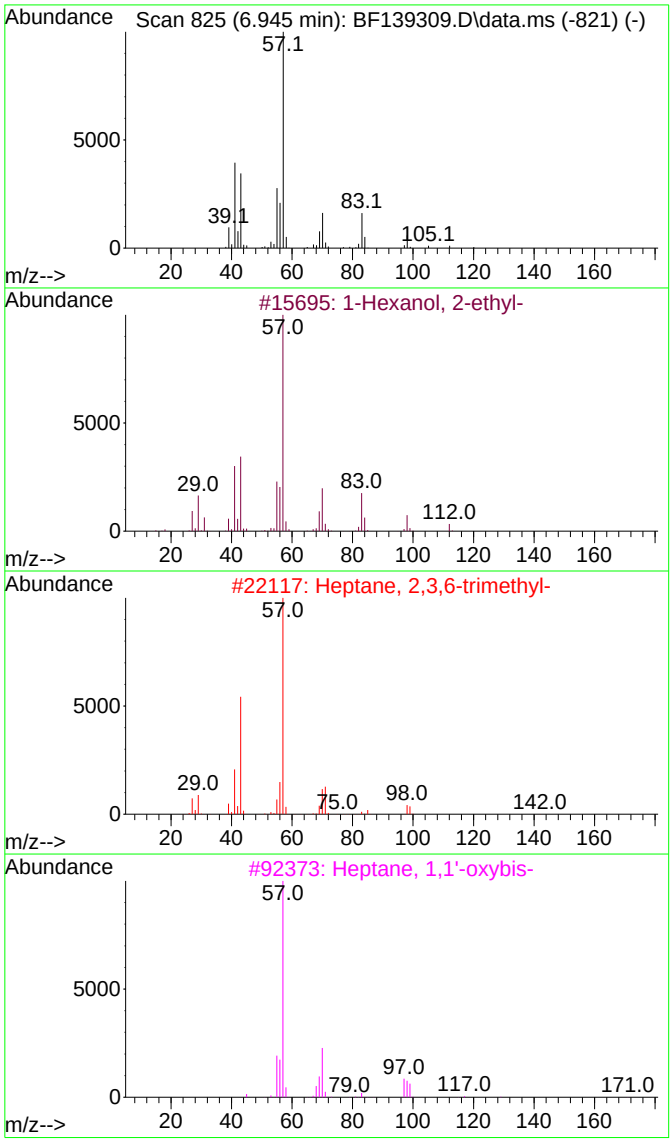
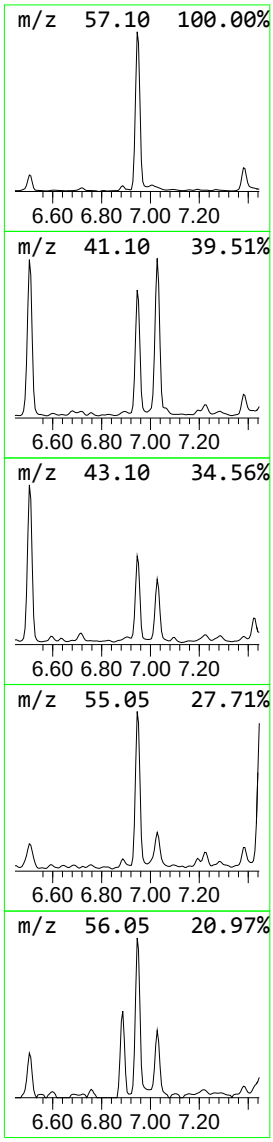
****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.945	5.42 ng	189344	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	45
5	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	45





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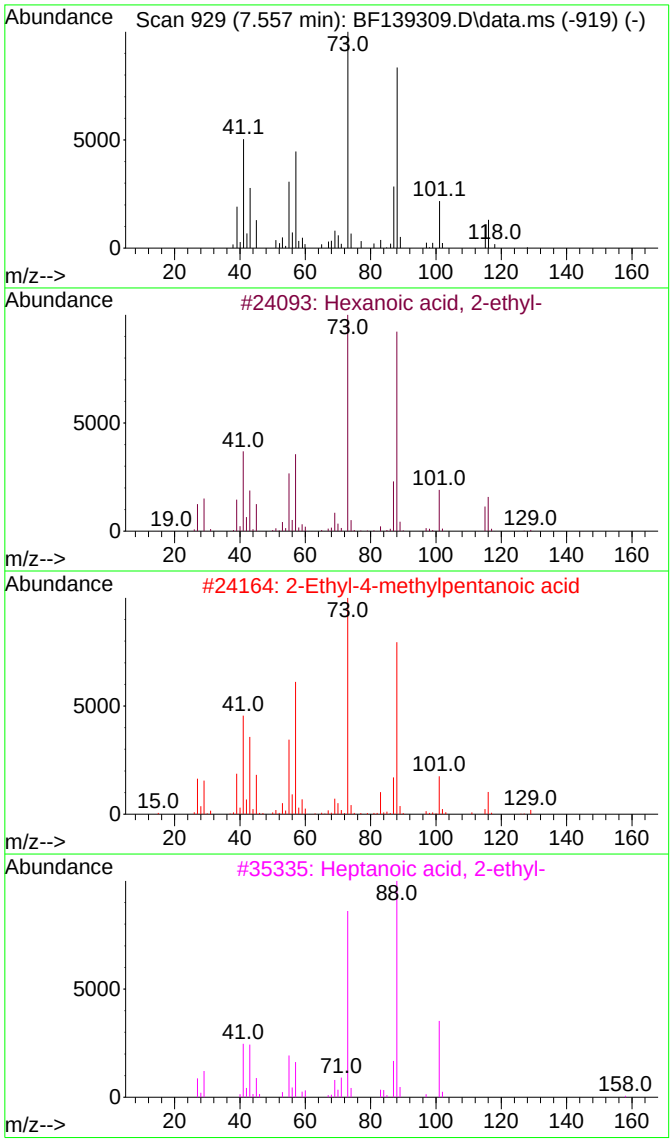
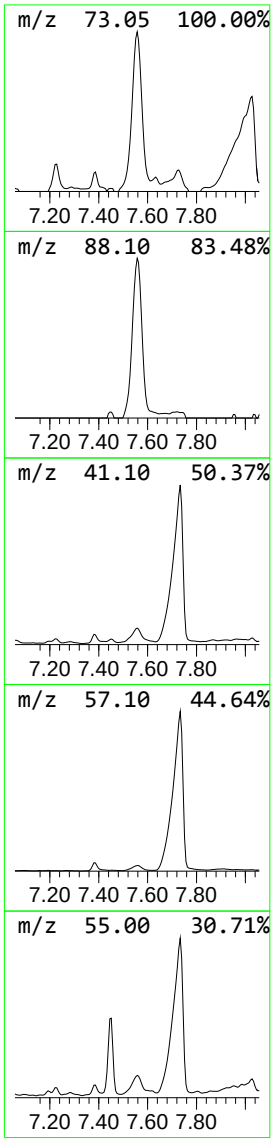
****

Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.557	3.42 ng	146642	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	78
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4	Butyl mannoside, tetramethyl ether	292	C14H28O6	1000501-84-1	50
5	1,4-Dioxane	88	C4H8O2	000123-91-1	47





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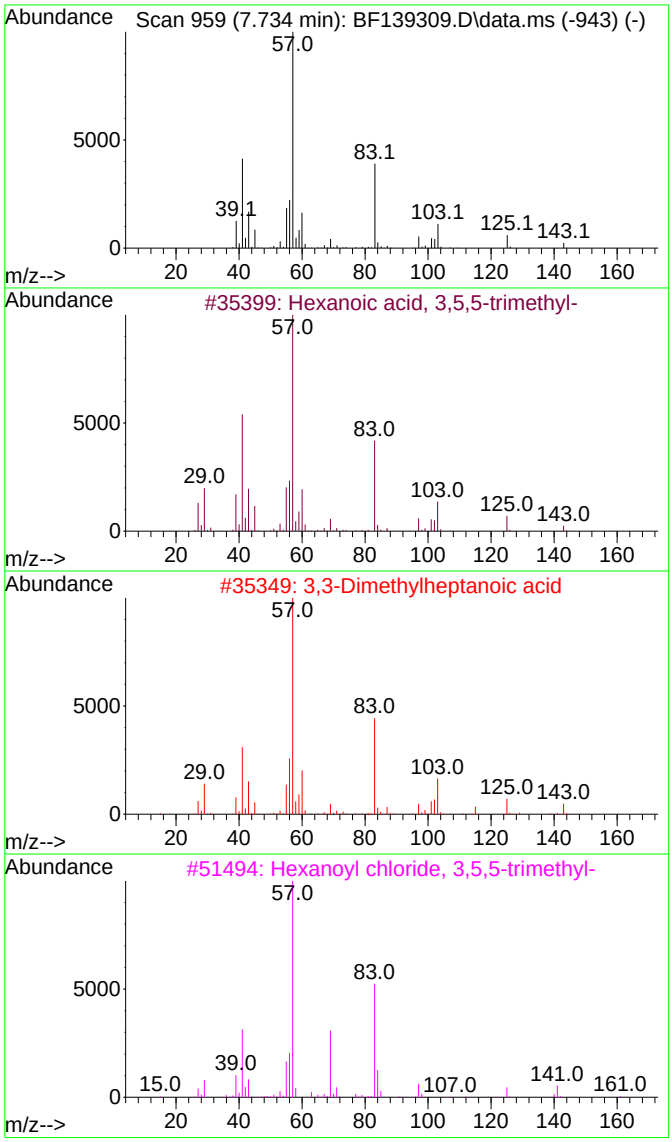
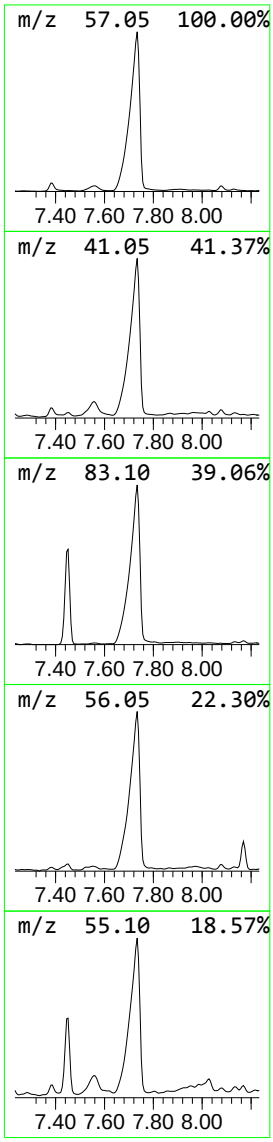
****
Peak Number 7 Hexanoic acid, 3,5,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.734	30.98 ng	1327240	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	53
4	6,6-Dimethylheptanoic acid	158	C9H18O2	015898-92-7	43
5	Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	32





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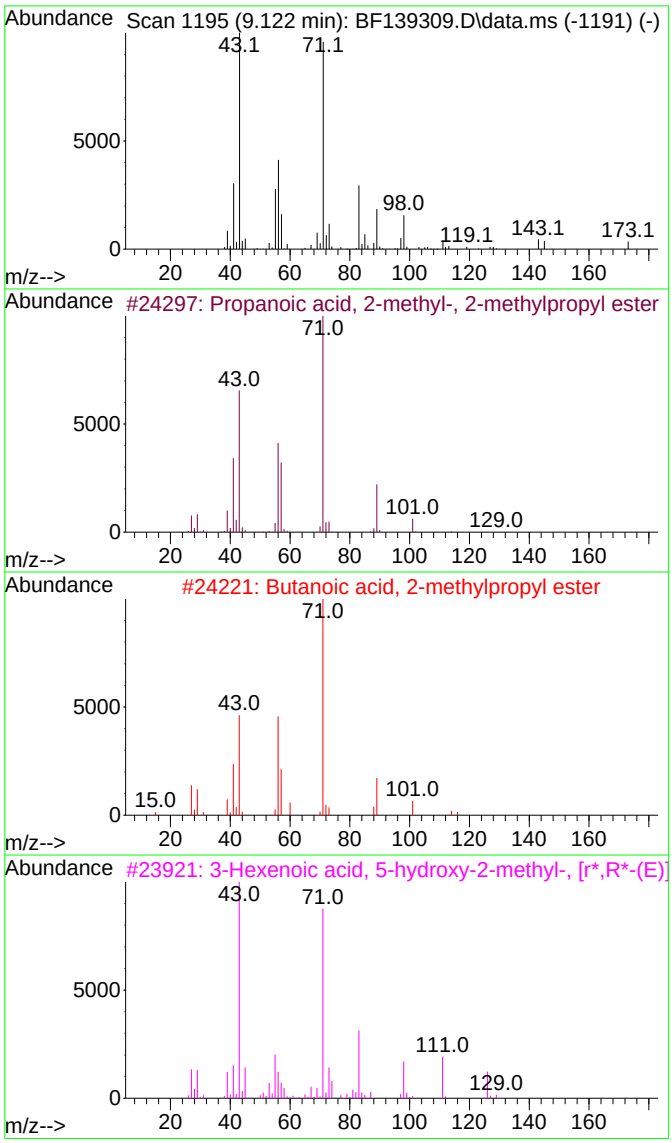
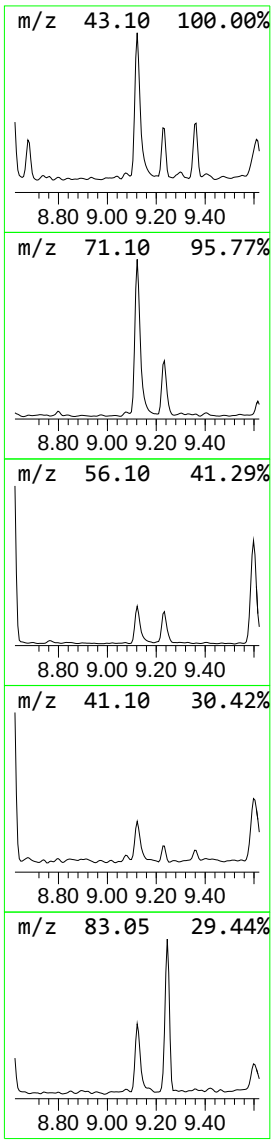
****
Peak Number 8 Propanoic acid, 2-methyl-, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.122	3.15 ng	138954	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	53
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	53
3	3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	40
4	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	38
5	Butanal isopentyl isopropyl acetal	202	C12H26O2	1000431-61-0	35





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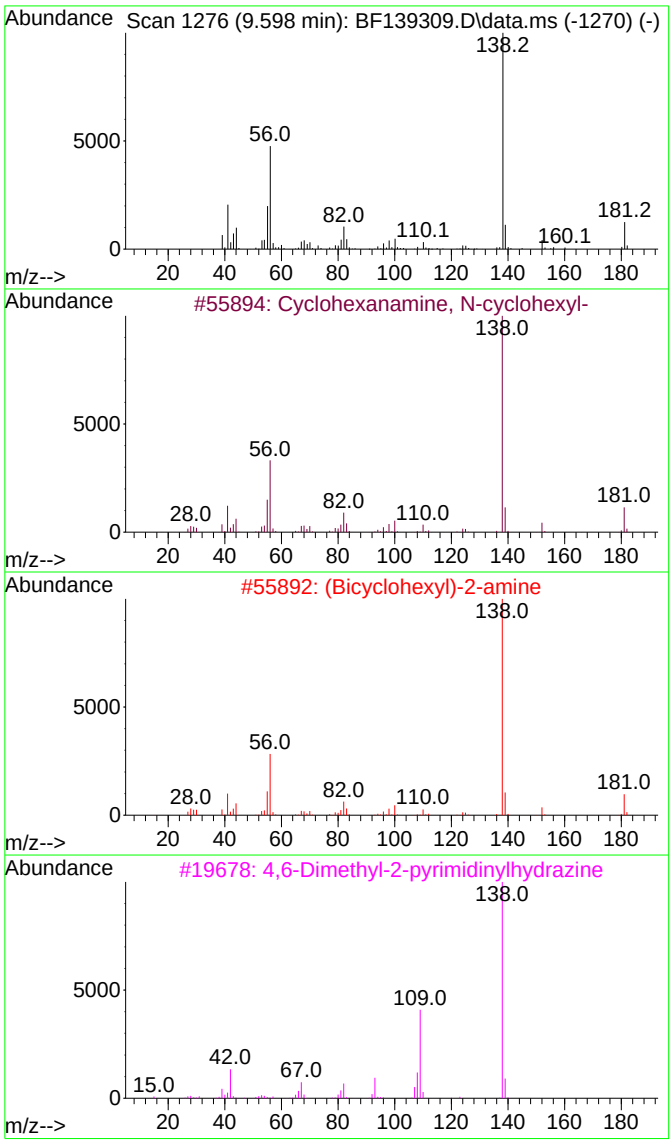
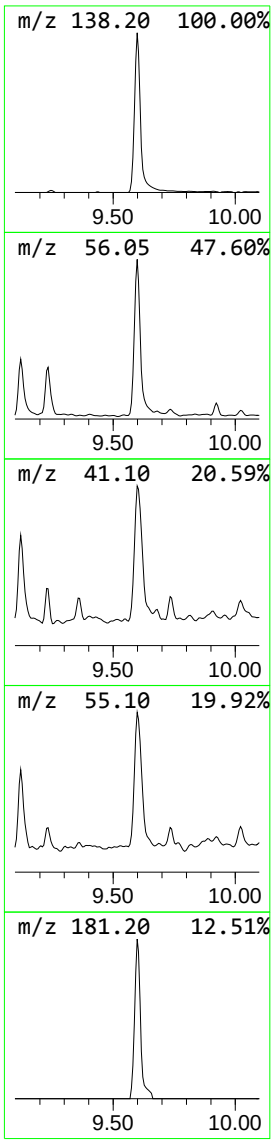
****
Peak Number 9 Cyclohexanamine, N-cyclohexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.598	6.64 ng	292914	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	96
2	(Bicyclohexyl)-2-amine	181	C12H23N	006283-14-3	95
3	4,6-Dimethyl-2-pyrimidinylhydrazine	138	C6H10N4	023906-13-0	43
4	(5R,8R)-8-Methyl-5-pentyloctahyd...	209	C14H27N	117959-79-2	43
5	N-[1-(Dicyclohexylamino)-2,2,2-t...	416	C19H30F6N2O	1000225-27-8	42





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Data File : BF139309.D
Acq On : 10 Sep 2024 20:00
Operator : RC/JU
Sample : P3853-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
252805

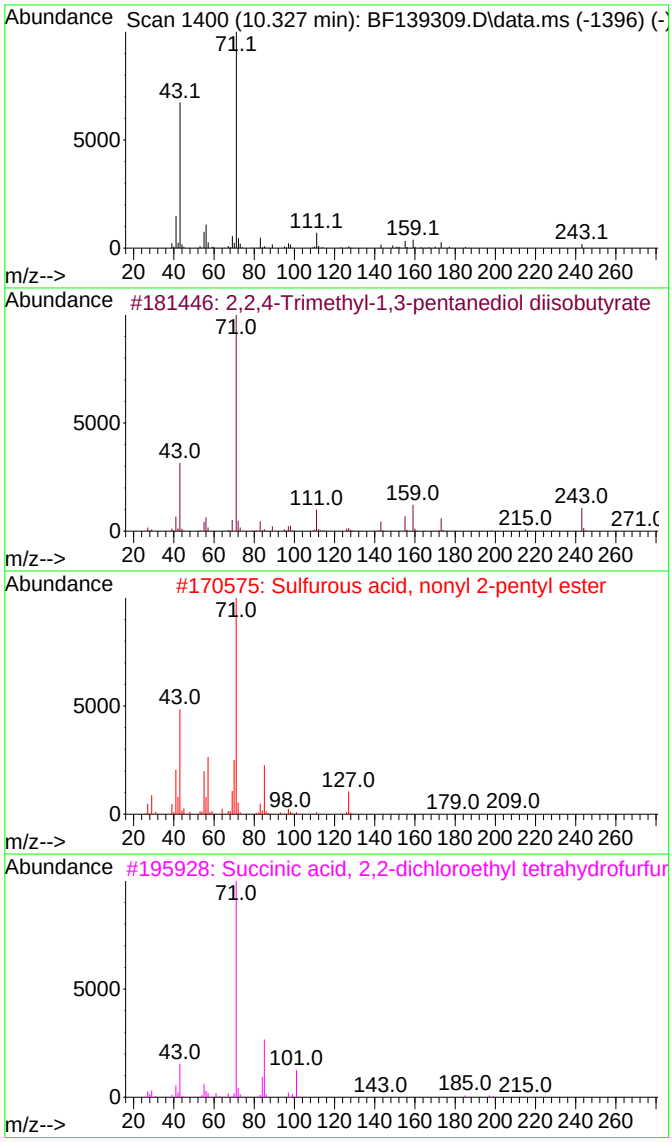
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

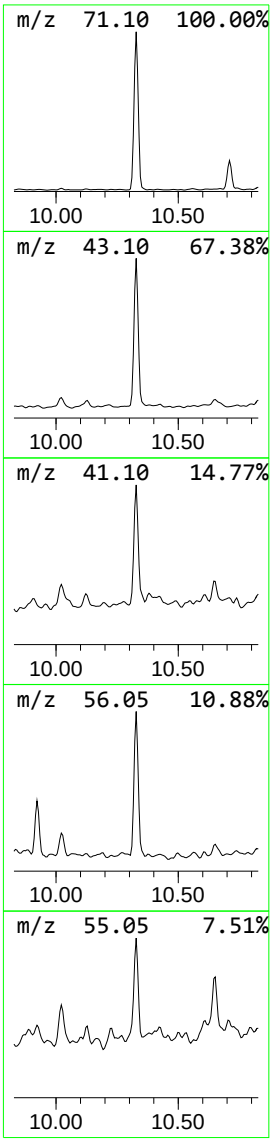
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	2.86 ng	126280	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	83
2	Sulfurous acid, nonyl 2-pentyl e...	278	C14H30O3S	1010309-15-8	50
3	Succinic acid, 2,2-dichloroethyl...	298	C11H16Cl2O5	1000390-71-6	45
4	Fumaric acid, nonyl tetrahydrofu...	326	C18H30O5	1000330-58-3	45
5	3-Cyclopentylpropionic acid, 2-t...	226	C13H22O3	1000293-46-9	42





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

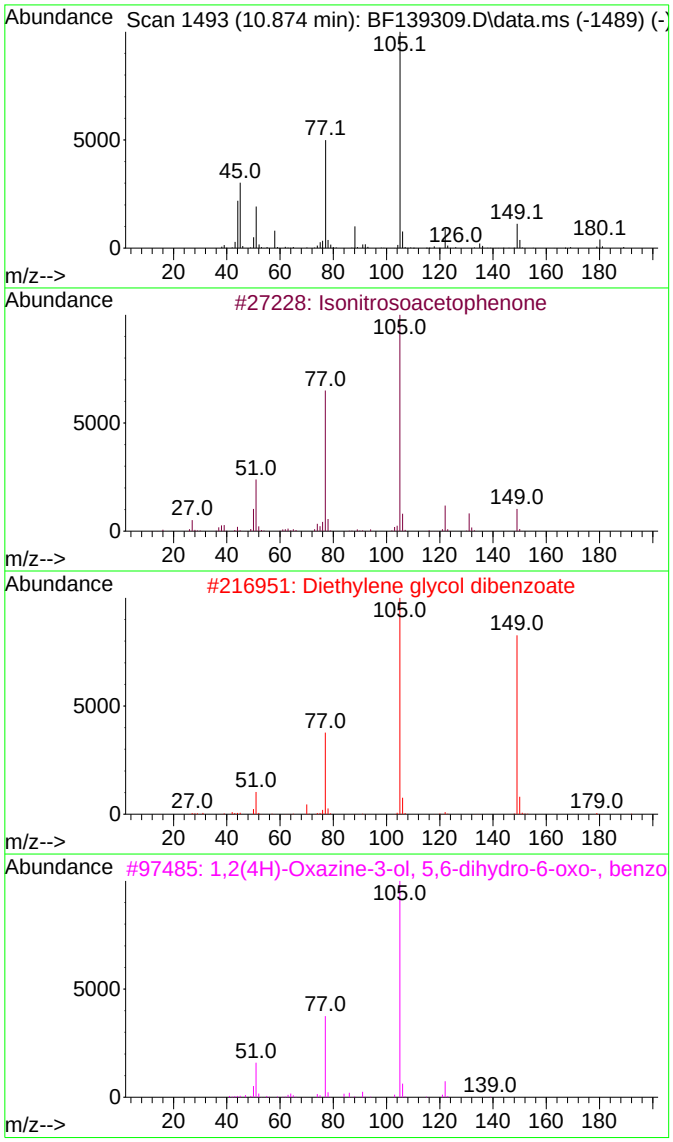
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

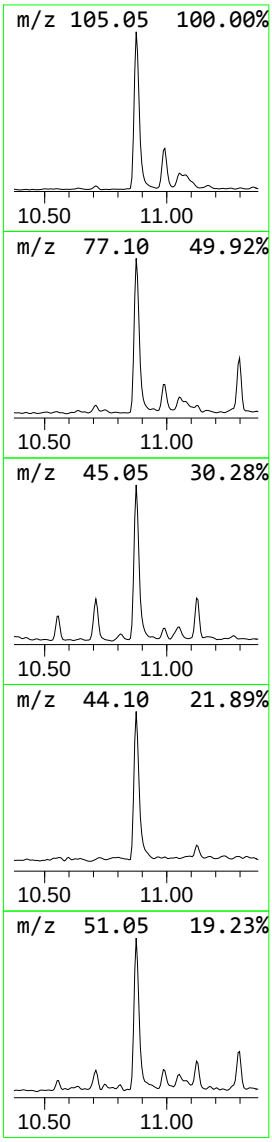
****

Peak Number 11 unknown10.874 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.874	5.24 ng	189450	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isonitrosoacetophenone	149	C8H7NO2	000532-54-7	49
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	43
3	1,2(4H)-Oxazine-3-ol, 5,6-dihydr...	219	C11H9NO4	1000253-25-6	43
4	Benzoylformic acid	150	C8H6O3	000611-73-4	43
5	Benzamide, N,N-dimethyl-	149	C9H11NO	000611-74-5	38





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Sample : P3853-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
252805

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

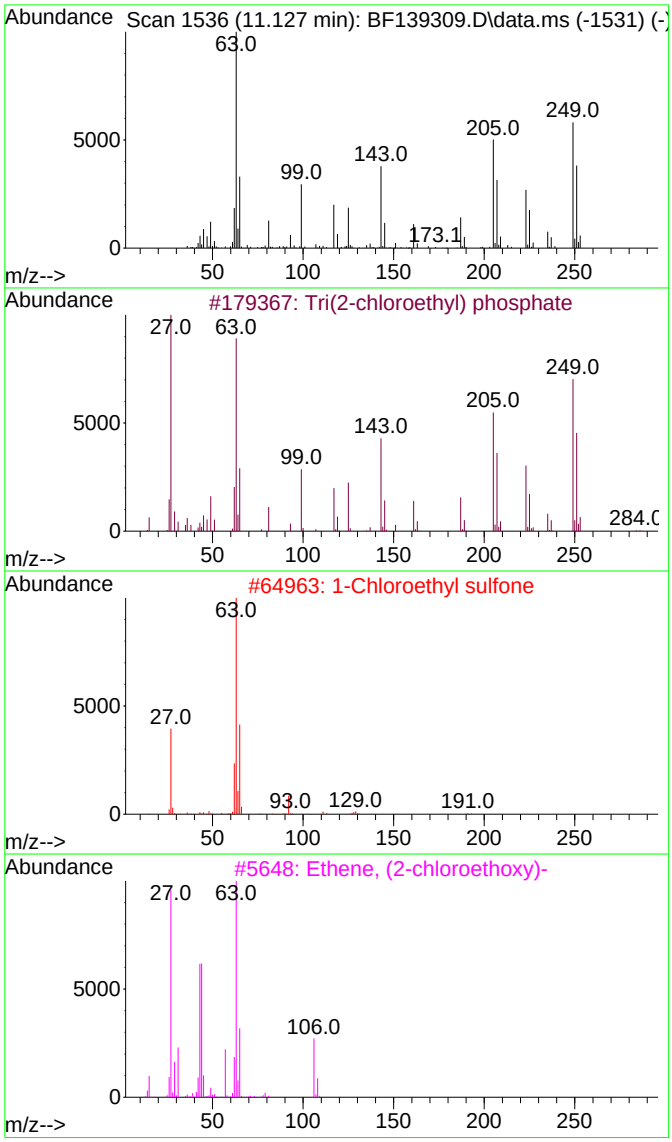
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

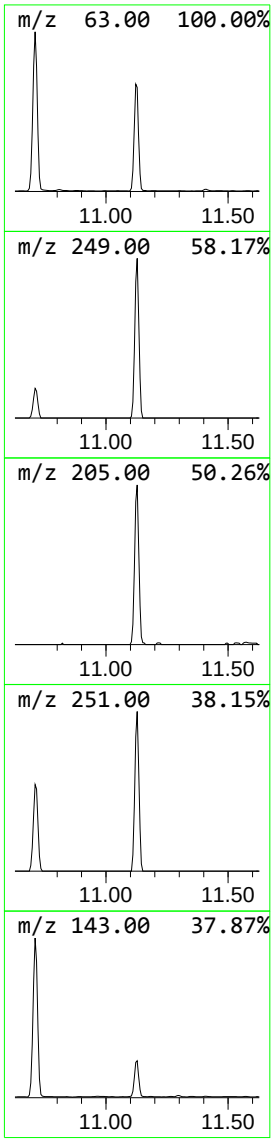
****

Peak Number 12 Tri(2-chloroethyl) phosphate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.127	8.29 ng	299575	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tri(2-chloroethyl) phosphate	284	C6H12Cl3O4P	000115-96-8	95
2	1-Chloroethyl sulfone	190	C4H8Cl2O2S	010038-07-0	47
3	Ethene, (2-chloroethoxy)-	106	C4H7ClO	000110-75-8	47
4	Oxalyl chloride	126	C2Cl2O2	000079-37-8	43
5	Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	38





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Sample : P3853-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
252805

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

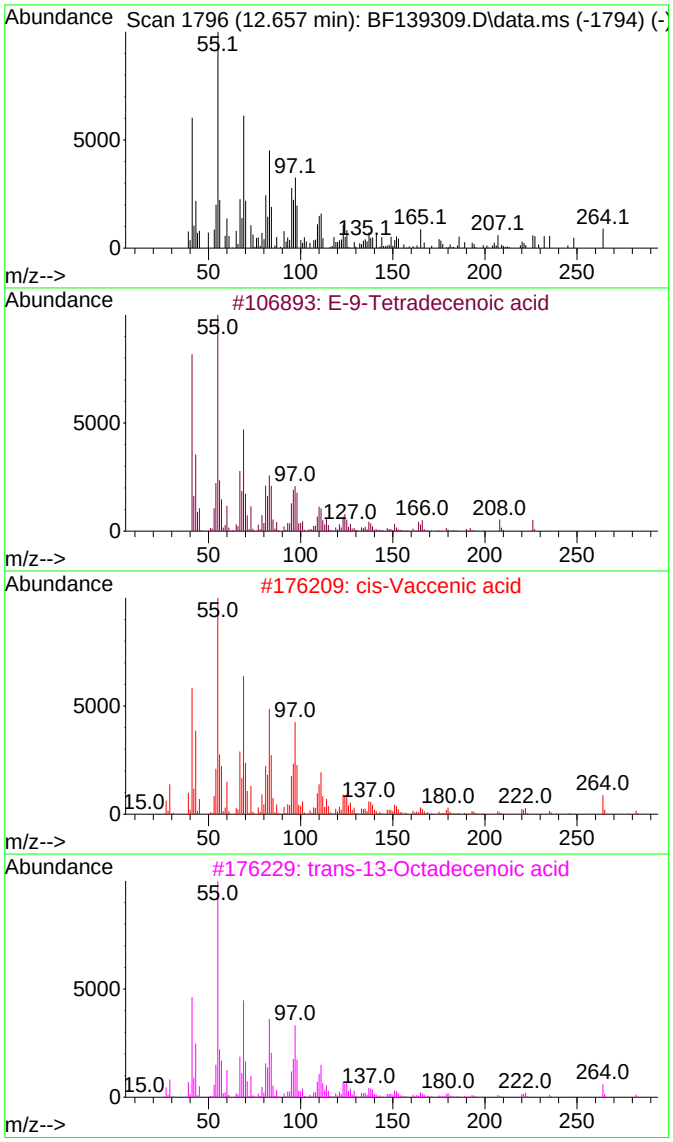
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

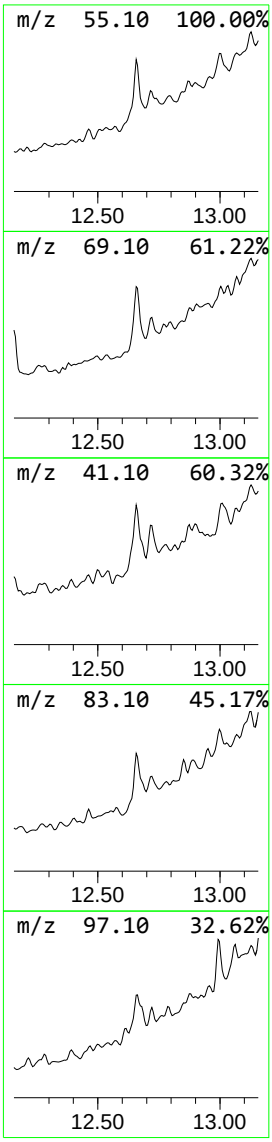
****

Peak Number 13 E-9-Tetradecenoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	2.13 ng	77143	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-9-Tetradecenoic acid	226	C14H26O2	050286-30-1	91
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	83
4	Oleic Acid	282	C18H34O2	000112-80-1	68
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139309.D
Acq On : 10 Sep 2024 20:00
Operator : RC/JU
Sample : P3853-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
252805

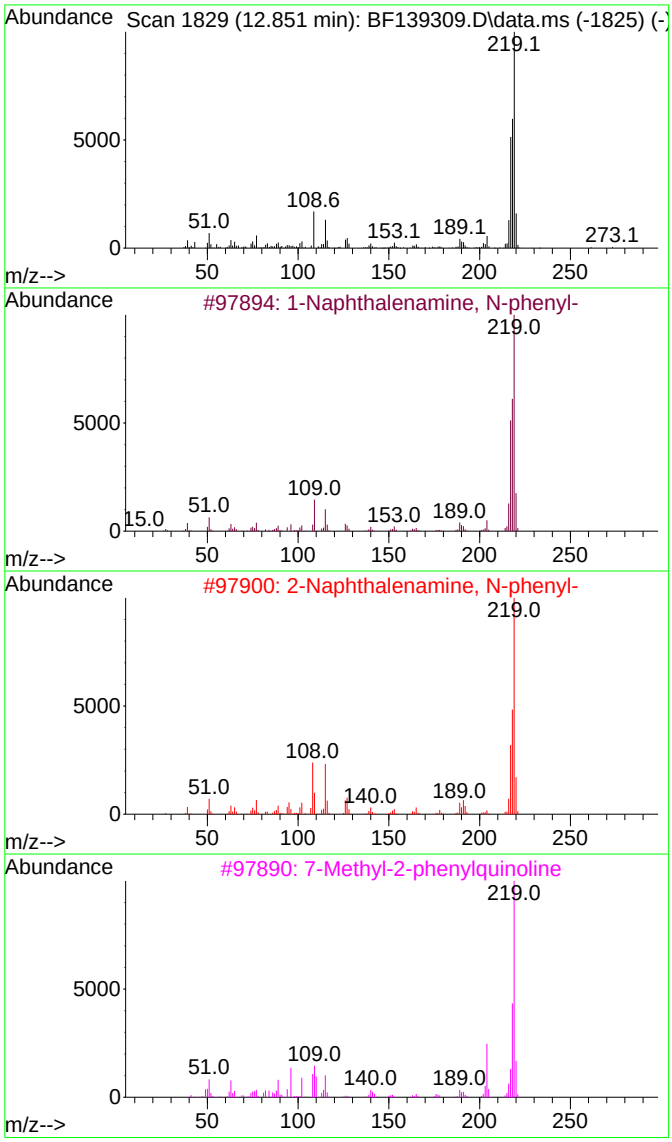
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

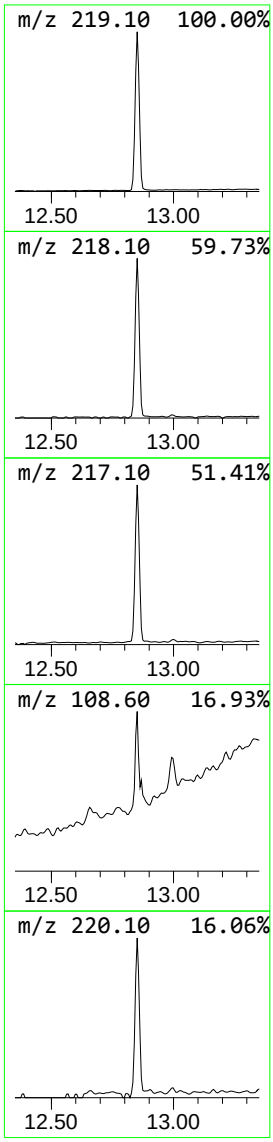
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 1-Naphthalenamine, N-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.851	12.78 ng	365186	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenamine, N-phenyl-	219	C16H13N	000090-30-2	98
2	2-Naphthalenamine, N-phenyl-	219	C16H13N	000135-88-6	89
3	7-Methyl-2-phenylquinoline	219	C16H13N	027356-39-4	64
4	Quinoline, 3-(4-methylphenyl)-	219	C16H13N	1000380-55-4	49
5	1,4-Methanonaphthalene, 1,4-dihy...	218	C17H14	055028-73-4	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139309.D
Acq On : 10 Sep 2024 20:00
Operator : RC/JU
Sample : P3853-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
252805

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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
Butane, 2-metho...	2.204	197.2	ng	6885270	1	6.887	698329	20.0
2-Pentanone, 4-...	5.104	5.4	ng	187764	1	6.887	698329	20.0
Pentanoic acid	5.645	7.8	ng	271711	1	6.887	698329	20.0
Ethanol, 2-butoxy-	5.834	17.5	ng	612472	1	6.887	698329	20.0
1-Hexanol, 2-et...	6.945	5.4	ng	189344	1	6.887	698329	20.0
Hexanoic acid, ...	7.557	3.4	ng	146642	2	8.169	856956	20.0
Hexanoic acid, ...	7.734	31.0	ng	1327240	2	8.169	856956	20.0
Propanoic acid,...	9.122	3.1	ng	138954	3	9.922	881801	20.0
Cyclohexanamine...	9.598	6.6	ng	292914	3	9.922	881801	20.0
2,2,4-Trimethyl...	10.328	2.9	ng	126280	3	9.922	881801	20.0
unknown10.874	10.874	5.2	ng	189450	4	11.410	723123	20.0
Tri(2-chloroeth...	11.127	8.3	ng	299575	4	11.410	723123	20.0
E-9-Tetradeceno...	12.657	2.1	ng	77143	4	11.410	723123	20.0
1-Naphthalenami...	12.851	12.8	ng	365186	5	14.045	571544	20.0