LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130379.D
Acq On : 22 Sep 2022 16:56
Operator : CG\JU
Sample : N4609-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DSN001

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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.834	464	467	477	rVB	113024	132243	3.42%	0.594%
2	5.263	536	540	552	rBV	1669936	1611625	41.68%	7.233%
3	5.398	559	563	575	rVB	260869	226493	5.86%	1.017%
4	6.151	688	691	695	rBV	56312	44857	1.16%	0.201%
5	6.298	712	716	732	rVB	968716	1033757	26.73%	4.640%
6	6.651	773	776	780	rBV	730715	659310	17.05%	2.959%
7	7.222	868	873	876	rVB	2048186	2161250	55.89%	9.700%
8	7.904	982	989	990	rBV2	64853	117609	3.04%	0.528%
9	7.934	990	994	998	rVV	931402	858963	22.21%	3.855%
10	8.075	1015	1018	1025	rVB3	27899	45264	1.17%	0.203%
11	8.310	1053	1058	1061	rBV	56426	83797	2.17%	0.376%
12	9.016	1172	1178	1181	rBV	4687099	3866877	100.00%	17.355%
13	9.686	1286	1292	1295	rBV	1059620	850693	22.00%	3.818%
14	9.851	1316	1320	1325	rBV	149028	172654	4.46%	0.775%
15	10.198	1375	1379	1382	rVB4	33721	51548	1.33%	0.231%
16	10.475	1422	1426	1434	rBV	2175190	1990527	51.48%	8.934%
17	10.933	1501	1504	1507	rBV	262958	211118	5.46%	0.948%
18	11.045	1518	1523	1525	rBV2	71359	68336	1.77%	0.307%
19	11.169	1540	1544	1547	rBV	768764	675115	17.46%	3.030%
20	11.333	1569	1572	1579	rVB4	34101	45126	1.17%	0.203%
21	11.569	1606	1612	1615	rBV3	57208	90502	2.34%	0.406%
22	11.710	1632	1636	1648	rVB	357648	382118	9.88%	1.715%
23	12.451	1758	1762	1766	rBV	2632522	2458462	63.58%	11.034%
24	12.492	1766	1769	1774	rVV2	54613	59271	1.53%	0.266%
25	12.680	1798	1801	1809	rVB	88594	88570	2.29%	0.398%
26	12.757	1809	1814	1817	rBV	3385499	2889878	74.73%	12.970%
27	13.798	1987	1991	1995	rBV	724014	604527	15.63%	2.713%
28	13.904	2004	2009	2013	rBV	226932	260278	6.73%	1.168%
29	15.192	2223	2228	2232	rVB	511597	539924	13.96%	2.423%

Sum of corrected areas: 22280692

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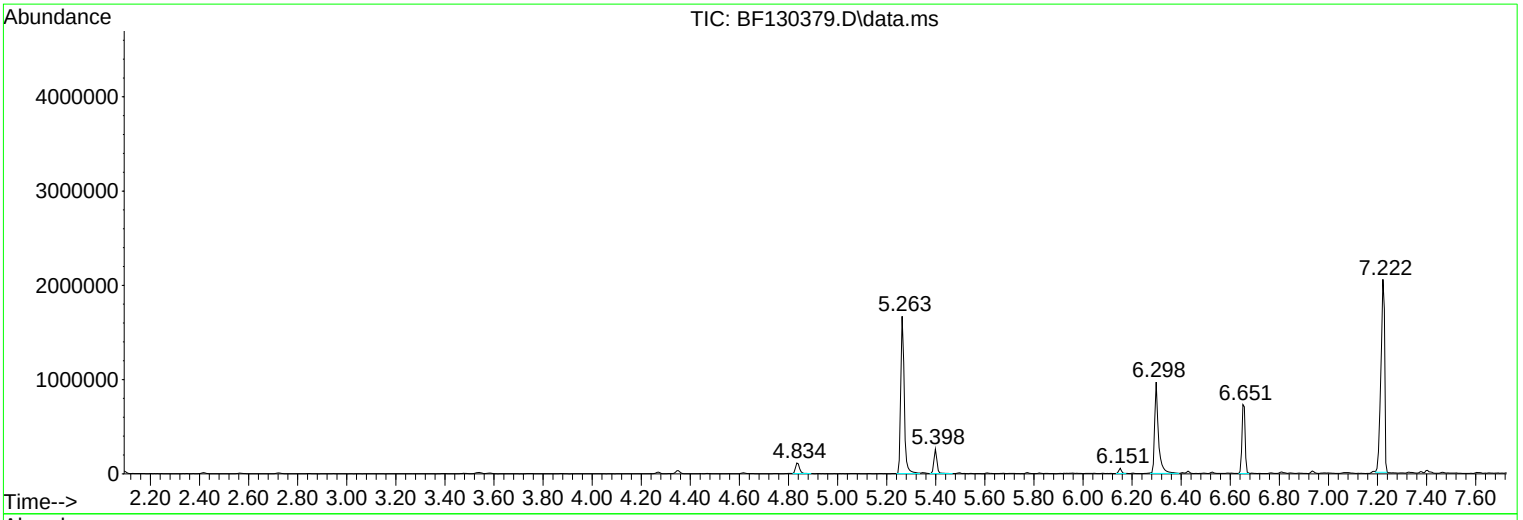
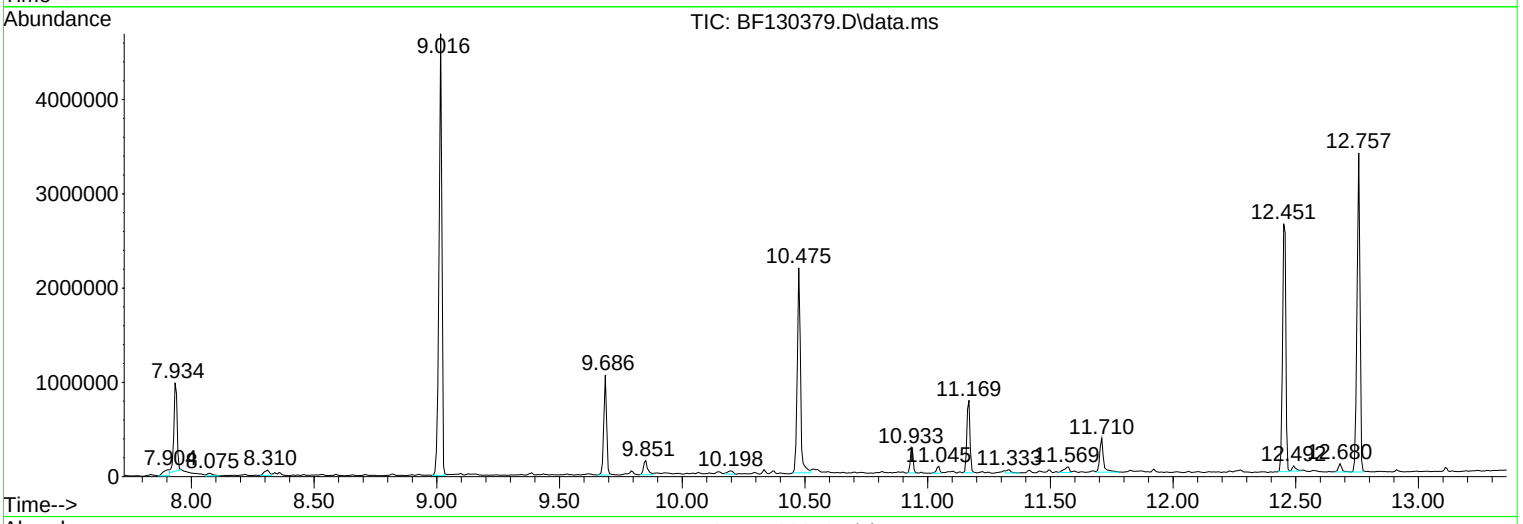
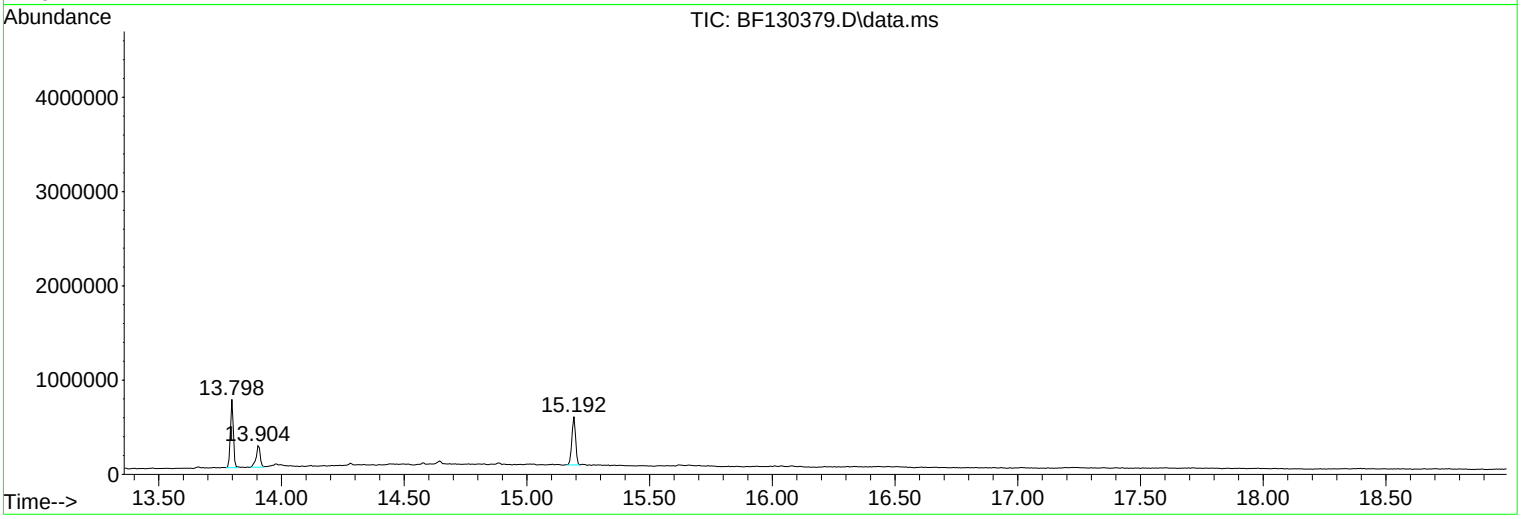
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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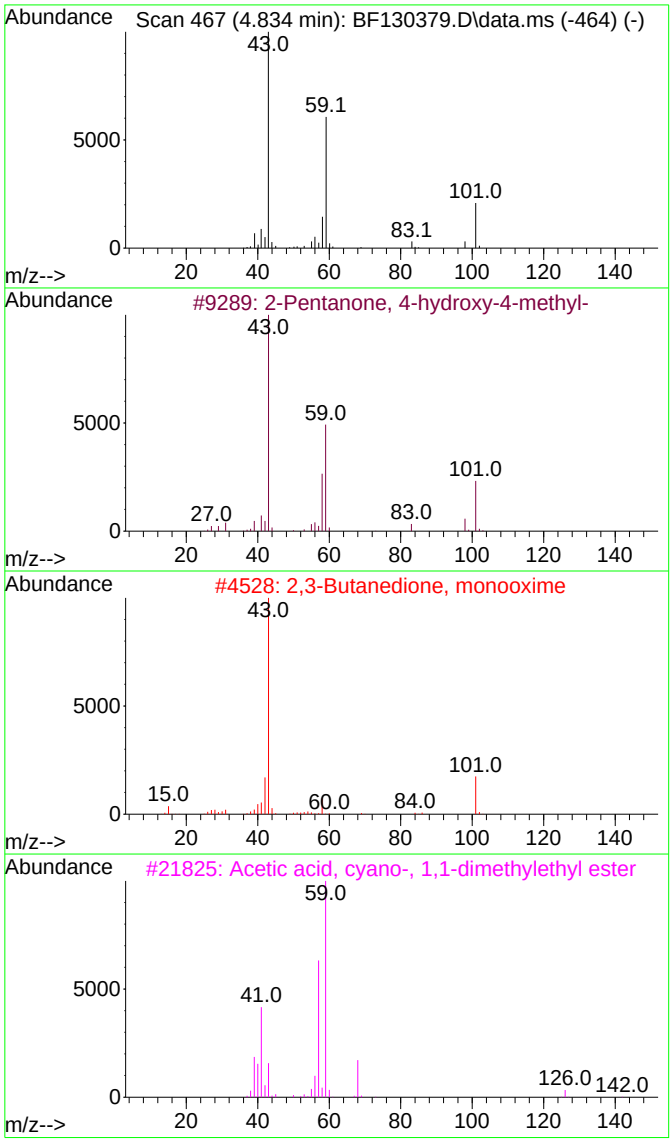
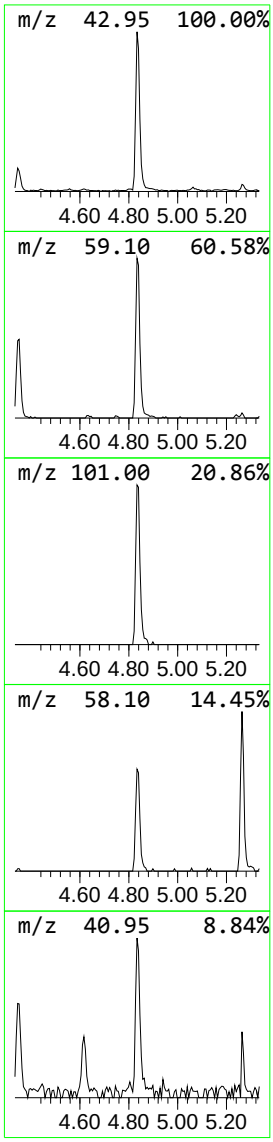
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.834	4.01 ng	132243	1,4-Dichlorobenzene-d4	6.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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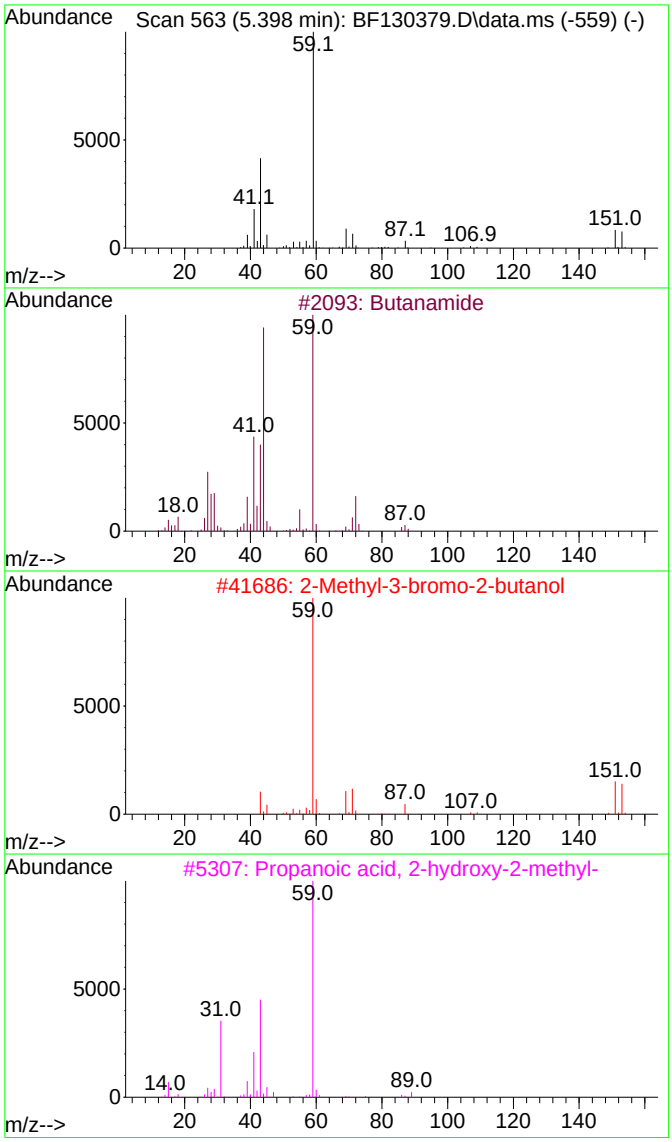
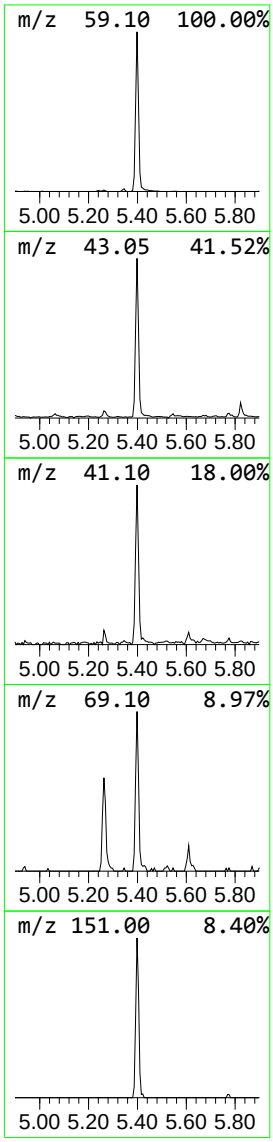
Peak Number 2 Butanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.398	6.87 ng	226493	1,4-Dichlorobenzene-d4	6.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanamide	87	C4H9NO	000541-35-5	72
2	2-Methyl-3-bromo-2-butanol	166	C5H11BrO	002588-77-4	72
3	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	64
4	4-Methyl-2-pentanol, methyl ether	116	C7H16O	1000333-93-5	50
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	42





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TIC Library : C:\Database\NIST20.L
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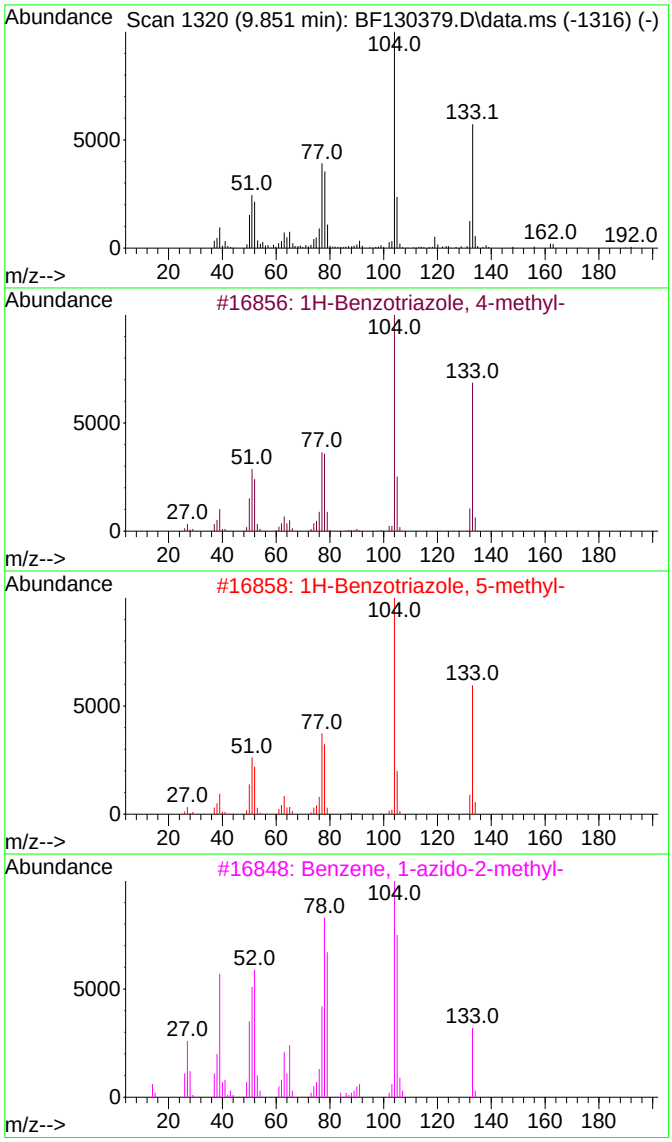
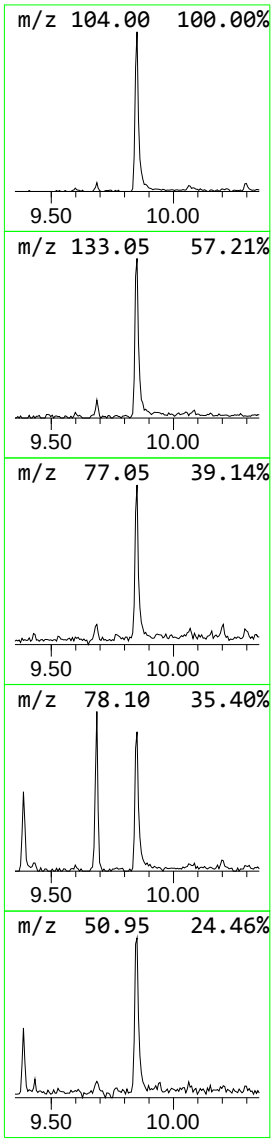
Peak Number 3 1H-Benzotriazole, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	4.06 ng	172654	Acenaphthene-d10	9.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	98
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	96
3	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	72
4	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	68
5	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	38





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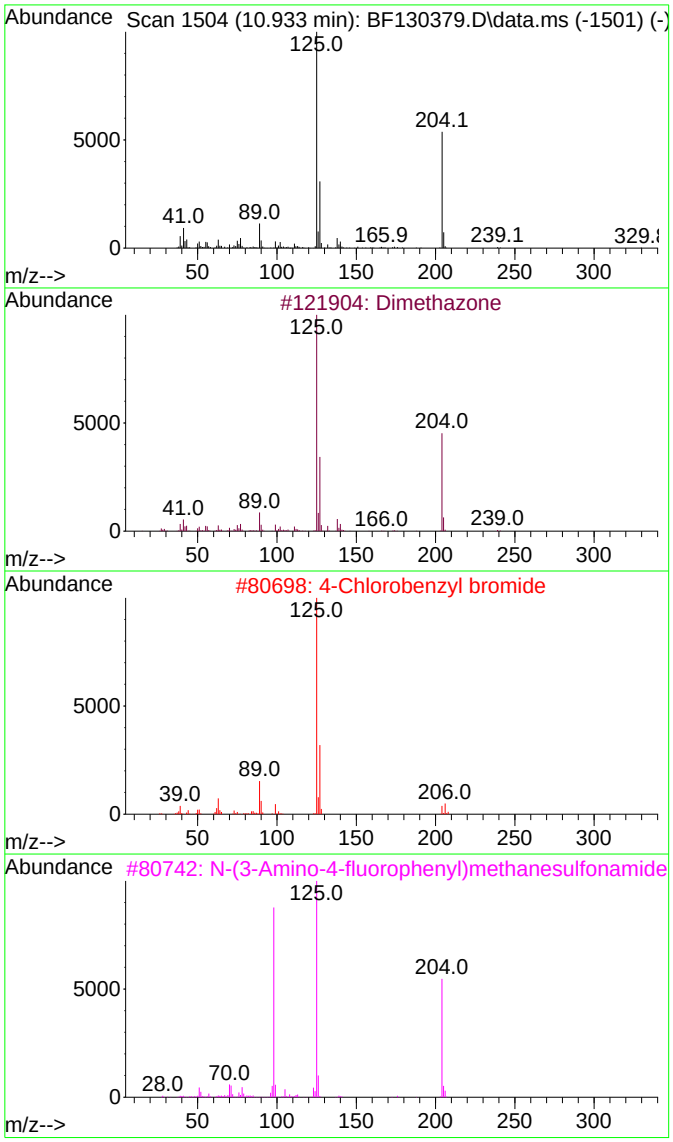
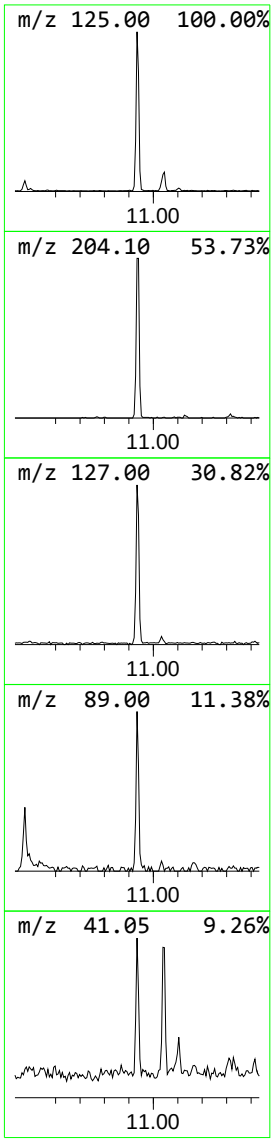
****

Peak Number 4 Dimethazone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.933	6.25 ng	211118	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethazone	239	C12H14ClNO2	081777-89-1	96
2	4-Chlorobenzyl bromide	204	C7H6BrCl	000622-95-7	70
3	N-(3-Amino-4-fluorophenyl)methan...	204	C7H9FN2O2S	926270-06-6	64
4	4-Acetamidophenyl-.alpha.-chloro...	323	C15H14ClNO3S	081269-17-2	53
5	N-(2-Chlorobenzyl)-1-propanamine	183	C10H14ClN	807343-03-9	53





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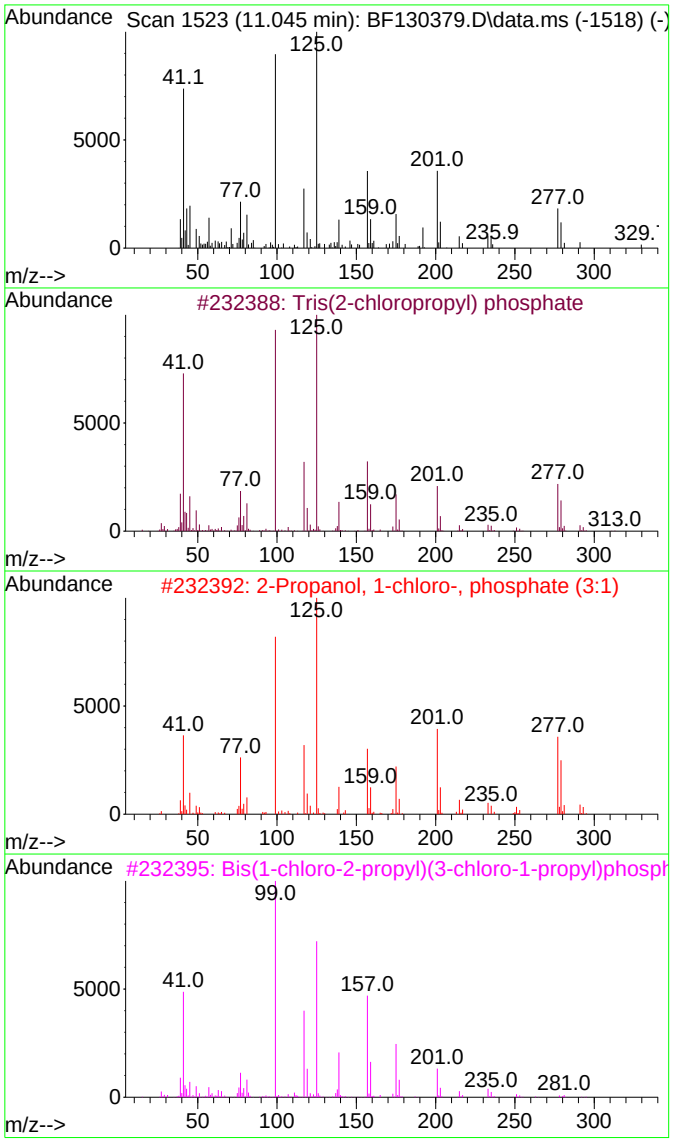
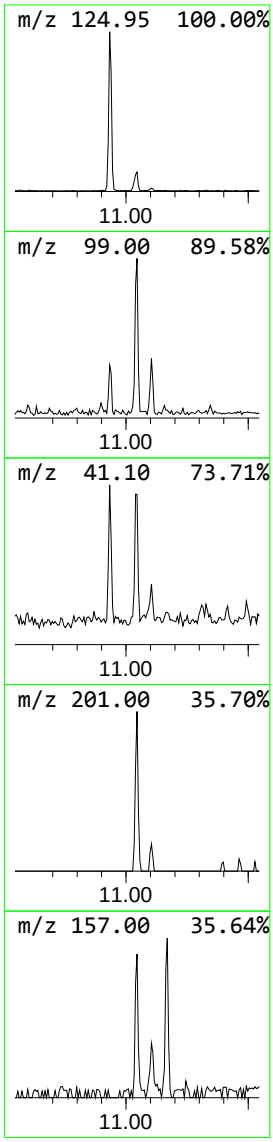
****
Peak Number 5 Tris(2-chloropropyl) phosphate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.045	2.02 ng	68336	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tris(2-chloropropyl) phosphate	326	C9H18Cl3O4P	006145-73-9	90
2	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	72
3	Bis(1-chloro-2-propyl)(3-chloro-...	326	C9H18Cl3O4P	137909-40-1	38
4	Benzoic acid, 4-[[2-(1-piperazin...	277	C14H19N3O3	1000350-32-6	25
5	Bis(3-chloro-1-propyl)(1-chloro-...	326	C9H18Cl3O4P	137888-35-8	22





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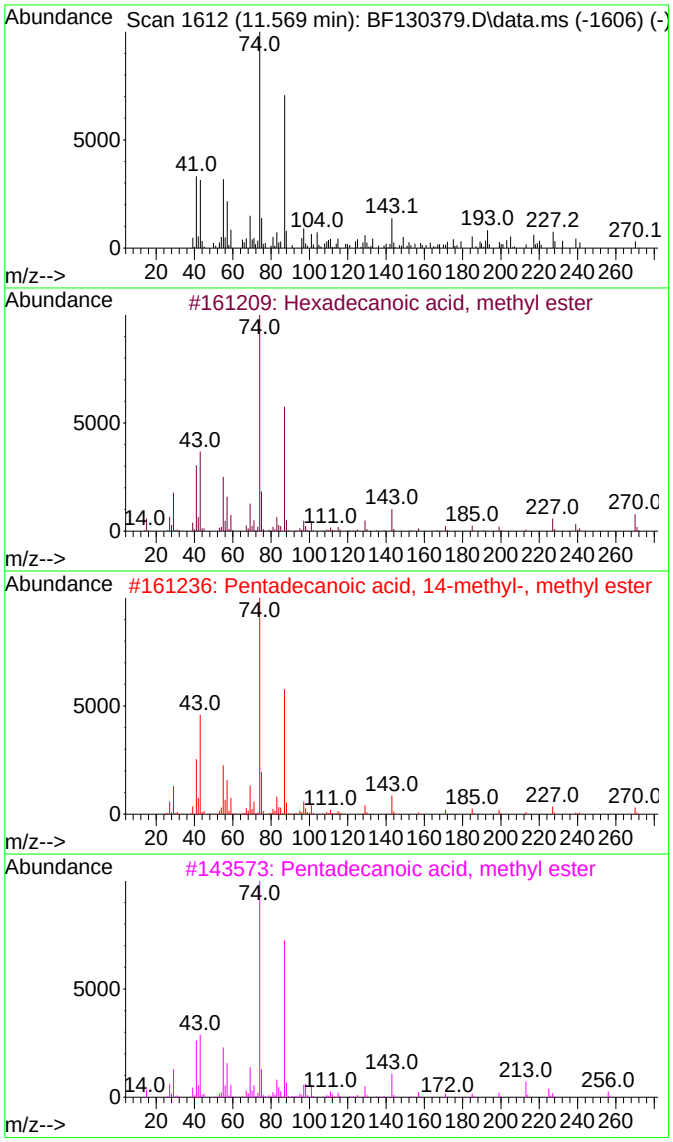
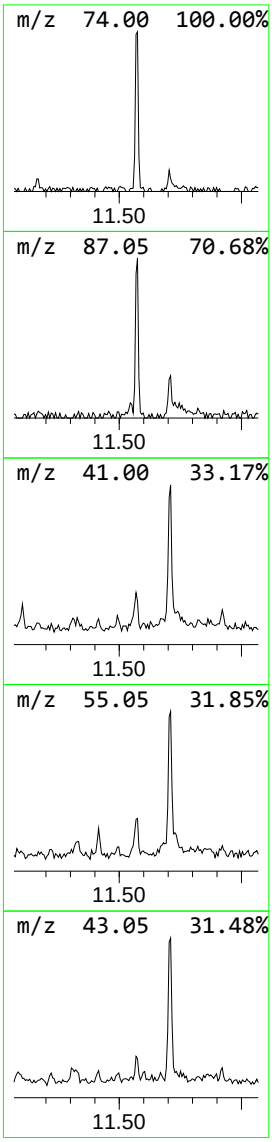
****
Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.569	2.68 ng	90502	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	72
5	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	72





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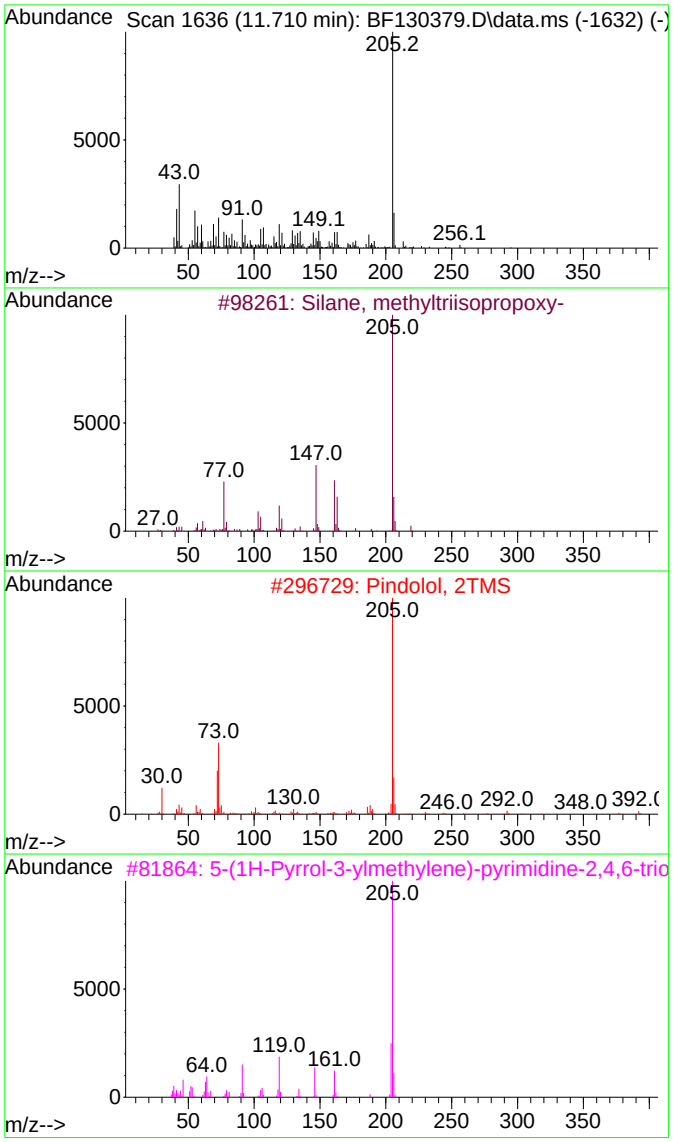
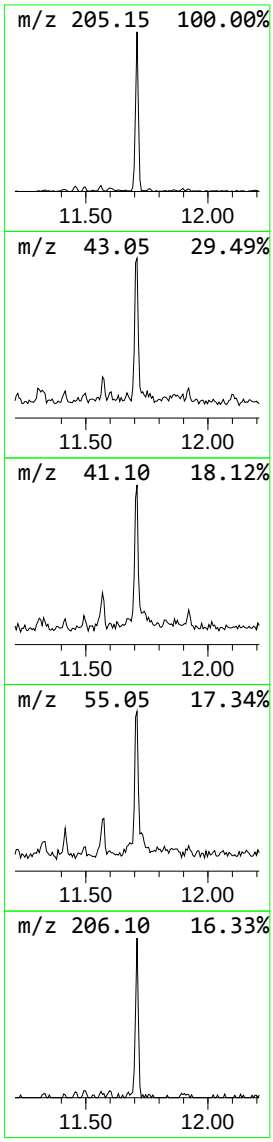
Peak Number 7 Silane, methyltriisopropoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.710	11.32 ng	382118	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, methyltriisopropoxy-	220	C10H24O3Si	1000416-18-8	53
2	Pindolol, 2TMS	392	C20H36N2O2Si2	1000408-11-5	53
3	5-(1H-Pyrrol-3-ylmethylene)-pyri...	205	C9H7N3O3	1000318-16-3	53
4	Succinic acid, di(2-ethylphenyl)...	326	C20H22O4	1000389-95-7	53
5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	50





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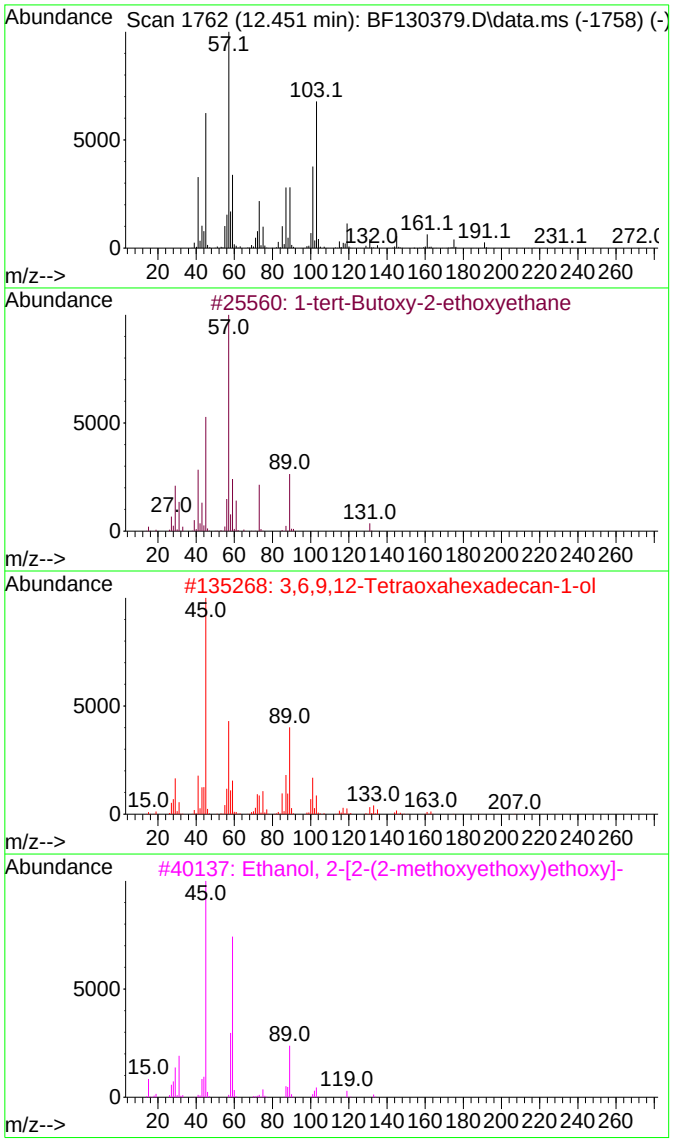
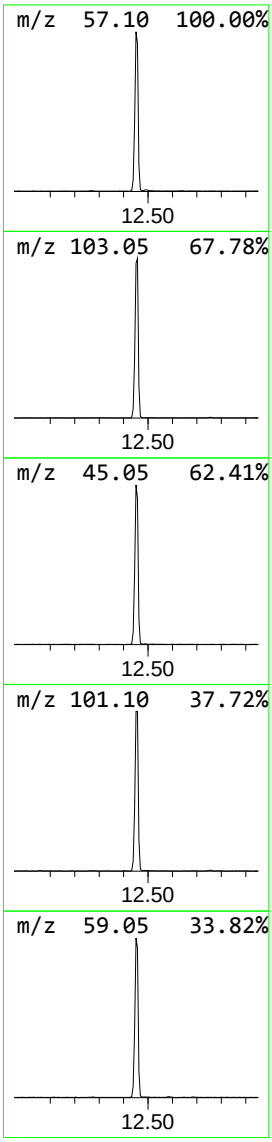
Peak Number 8 unknown12.451 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.451	72.83 ng	2458460	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43
2	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	35
3	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	35
4	2-[2-[2-[2-[2-[2-(2-Methoxyet...	384	C17H36O9	025990-96-9	35
5	3,3-Diethoxy-1-propanol, propyl ...	190	C10H22O3	1000395-37-1	35





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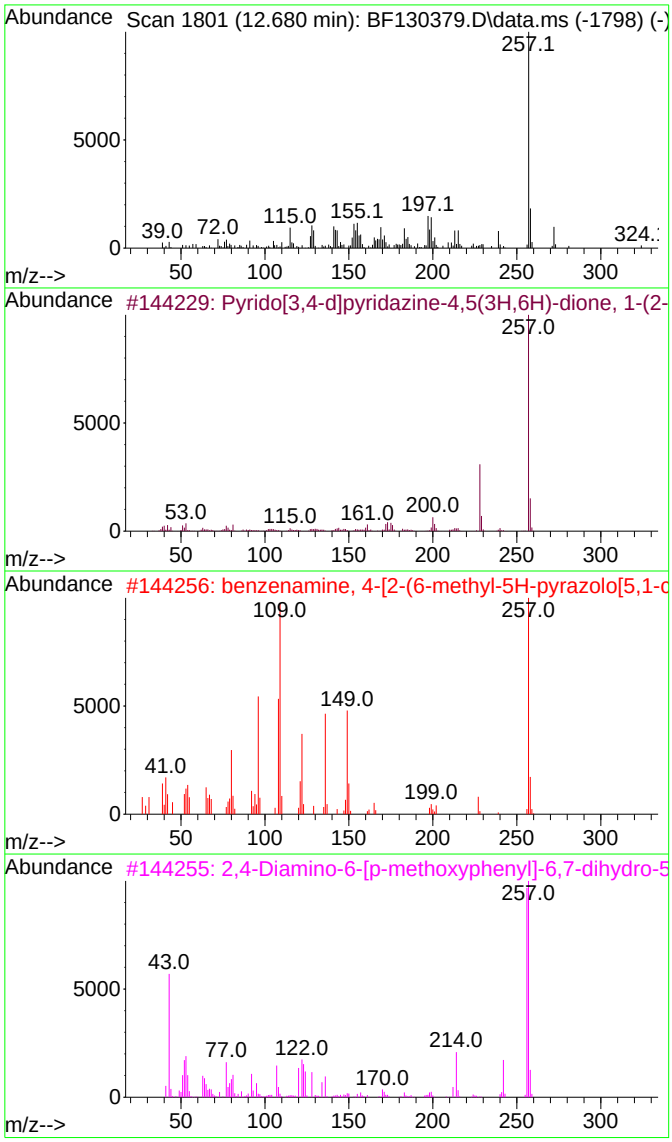
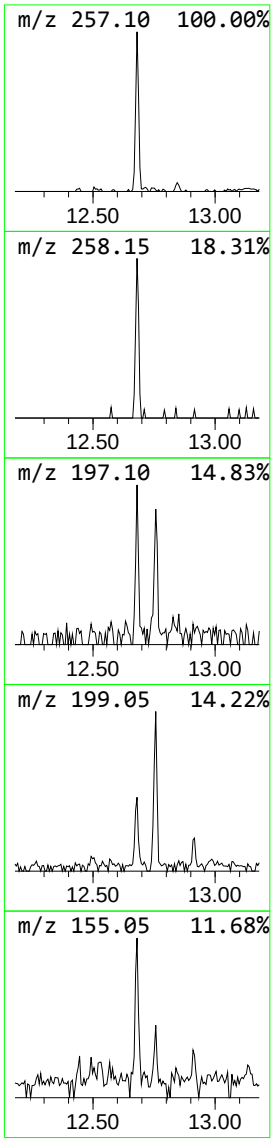
Peak Number 9 unknown12.680 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.93 ng	88570	Chrysene-d12	13.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrido[3,4-d]pyridazine-4,5(3H,6...	257	C13H11N3O3	160033-05-6	49
2	benzenamine, 4-[2-(6-methyl-5H-p...	257	C13H15N5O	1000396-74-3	47
3	2,4-Diamino-6-[p-methoxyphenyl]-...	257	C13H15N5O	1000251-46-9	47
4	6,7-Dimethoxy-2-trifluoromethylq...	257	C12H10F3NO2	041192-91-0	47
5	Benz[c]acridine, 7,9-dimethyl-	257	C19H15N	000963-89-3	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130379.D
Acq On : 22 Sep 2022 16:56
Operator : CG\JU
Sample : N4609-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

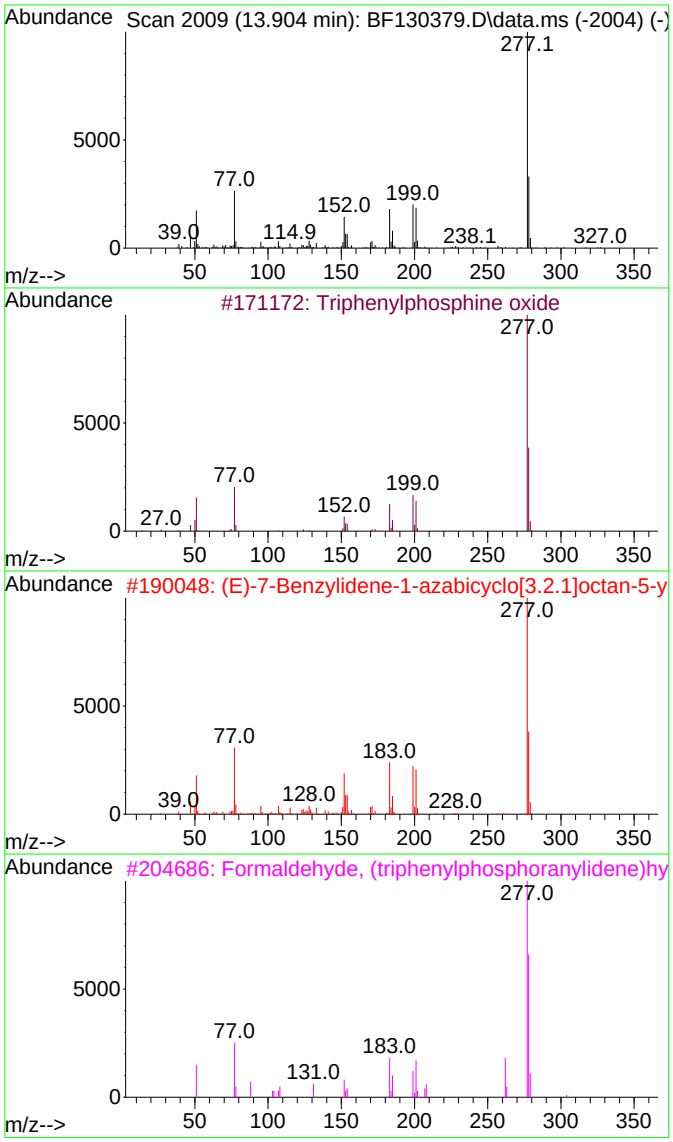
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

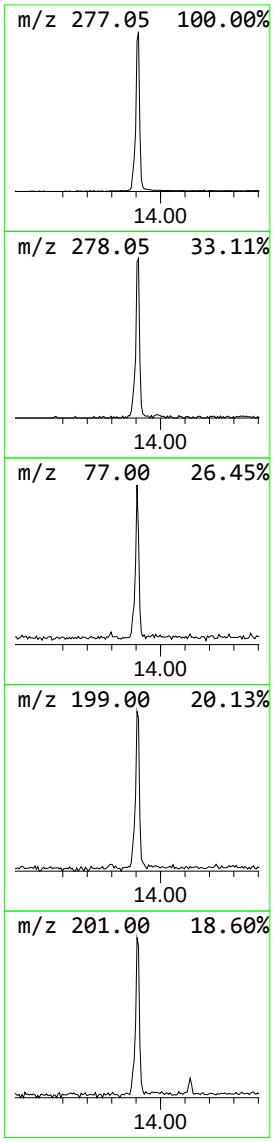
****

Peak Number 10 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	8.61 ng	260278	Chrysene-d12	13.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	94
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	59
4	Benzoic acid, 2-(diphenylphosphi...	306	C19H15O2P	017261-28-8	50
5	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130379.D
Acq On : 22 Sep 2022 16:56
Operator : CG\JU
Sample : N4609-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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-...	4.834	4.0	ng	132243	1	6.657	659310	20.0
Butanamide	5.398	6.9	ng	226493	1	6.657	659310	20.0
1H-Benzotriazol...	9.851	4.1	ng	172654	3	9.686	850693	20.0
Dimethazone	10.933	6.3	ng	211118	4	11.169	675115	20.0
Tris(2-chloropr...	11.045	2.0	ng	68336	4	11.169	675115	20.0
Hexadecanoic ac...	11.569	2.7	ng	90502	4	11.169	675115	20.0
Silane, methylt...	11.710	11.3	ng	382118	4	11.169	675115	20.0
unknown12.451	12.451	72.8	ng	2458460	4	11.169	675115	20.0
unknown12.680	12.680	2.9	ng	88570	5	13.798	604527	20.0
Triphenylphosph...	13.904	8.6	ng	260278	5	13.798	604527	20.0