

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071924\
 Data File : BF138588.D
 Acq On : 19 Jul 2024 14:28
 Operator : RC/JU
 Sample : P3246-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-CTW2-BL-01

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-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	19	rVB	1123059	1719232	100.00%	12.082%
2	3.381	214	219	236	rBV	13667	41195	2.40%	0.289%
3	5.075	502	507	515	rVB	76733	113600	6.61%	0.798%
4	5.481	571	576	588	rBV	1164741	1503181	87.43%	10.563%
5	6.493	742	748	753	rBV	1189904	1565458	91.06%	11.001%
6	6.857	805	810	815	rVB	344626	416447	24.22%	2.926%
7	7.416	899	905	910	rBV	776023	1002565	58.31%	7.045%
8	7.669	943	948	955	rBV	19245	25115	1.46%	0.176%
9	8.139	1022	1028	1033	rBV	436972	550054	31.99%	3.865%
10	8.451	1076	1081	1095	rBV	38451	58642	3.41%	0.412%
11	9.210	1204	1210	1215	rBV	1244939	1579400	91.87%	11.099%
12	9.892	1320	1326	1331	rBV	503737	621592	36.16%	4.368%
13	9.986	1336	1342	1348	rBV	40682	62164	3.62%	0.437%
14	10.298	1387	1395	1401	rBV3	15706	34884	2.03%	0.245%
15	10.680	1454	1460	1475	rBV	836684	1072555	62.39%	7.537%
16	11.375	1573	1578	1584	rBV	532277	665098	38.69%	4.674%
17	11.898	1662	1667	1681	rBV2	108452	189600	11.03%	1.332%
18	12.686	1796	1801	1809	rBV	30196	56701	3.30%	0.398%
19	12.851	1827	1829	1834	rVB	14677	17278	1.00%	0.121%
20	12.957	1842	1847	1853	rBV	1219586	1605448	93.38%	11.282%
21	13.186	1882	1886	1890	rBV	19092	24177	1.41%	0.170%
22	13.527	1940	1944	1953	rVB2	26151	43179	2.51%	0.303%
23	13.857	1995	2000	2015	rVB	78027	148724	8.65%	1.045%
24	14.010	2021	2026	2036	rVB	355622	473905	27.56%	3.330%
25	14.169	2049	2053	2064	rBV	26913	37958	2.21%	0.267%
26	14.474	2101	2105	2111	rBV	30211	46081	2.68%	0.324%
27	14.780	2153	2157	2164	rVB	26331	34496	2.01%	0.242%
28	15.115	2210	2214	2219	rBV	26092	36863	2.14%	0.259%
29	15.474	2270	2275	2288	rVB	285661	463375	26.95%	3.256%
30	15.927	2349	2352	2357	rVB2	13914	21250	1.24%	0.149%

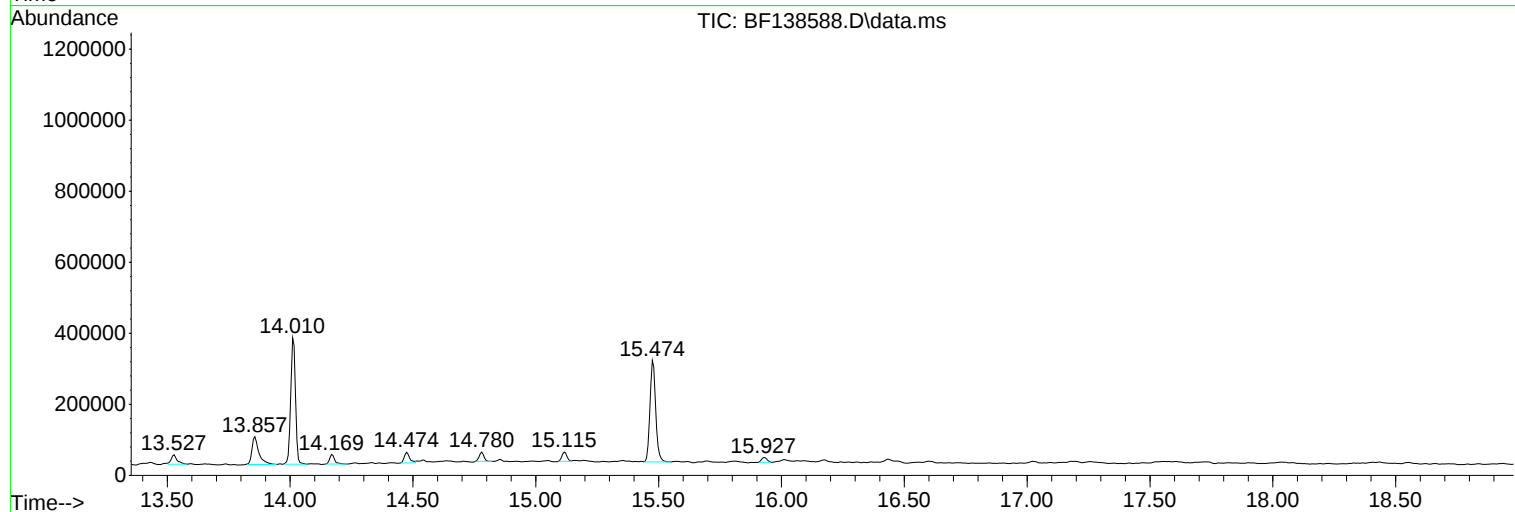
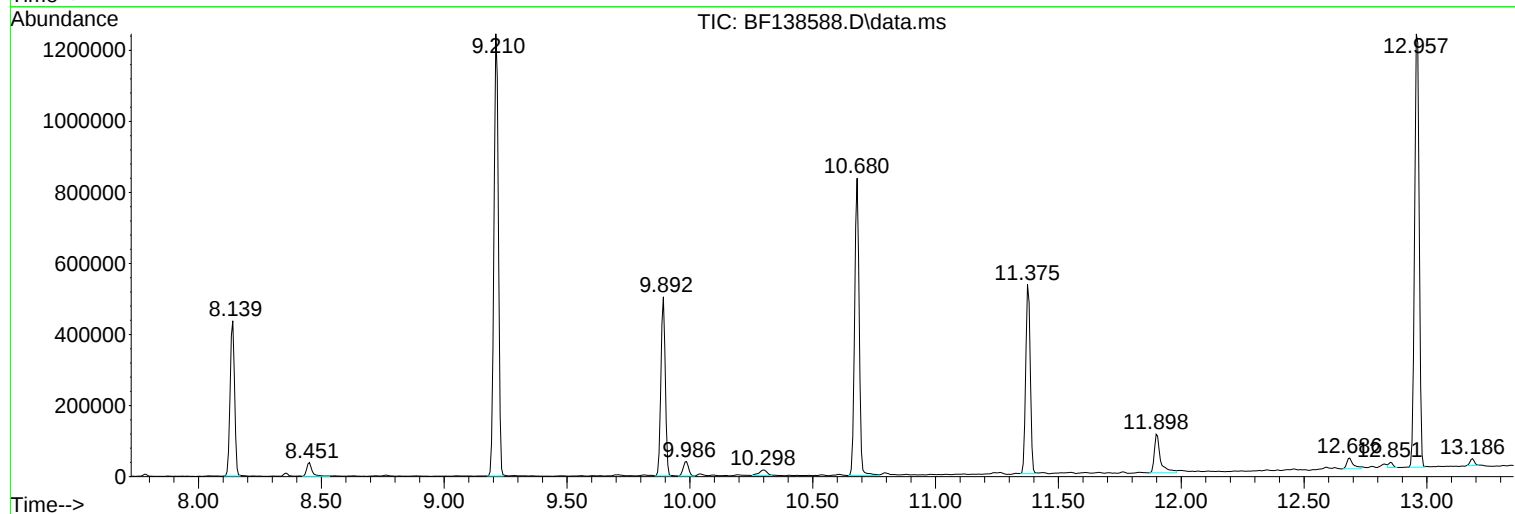
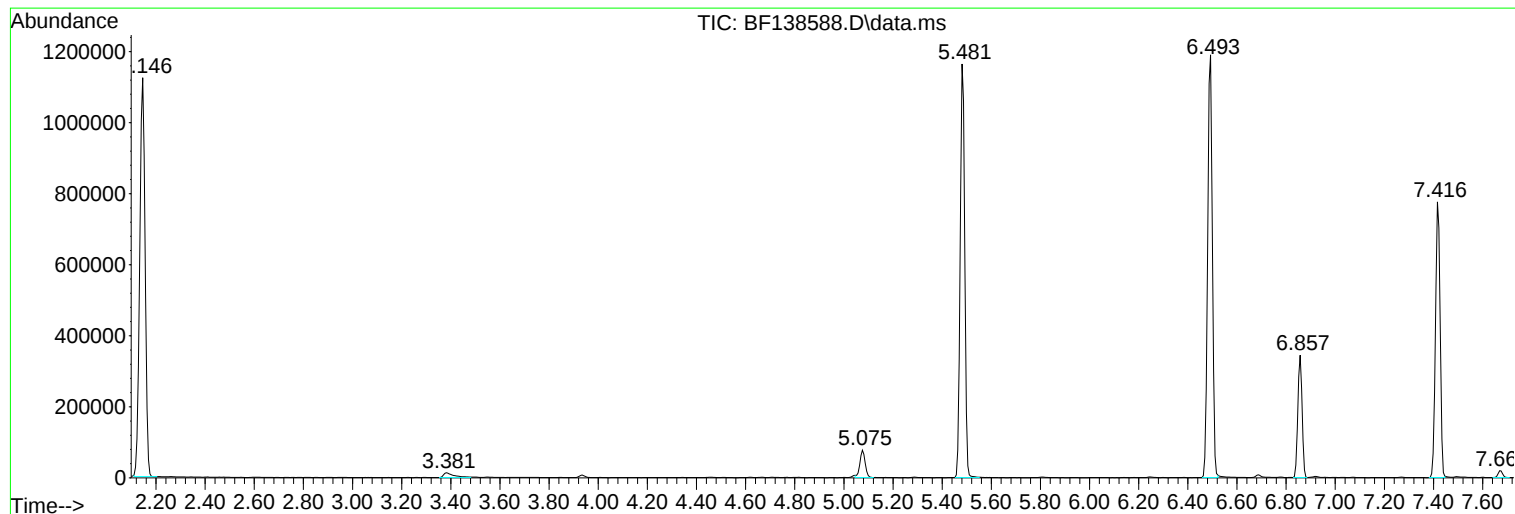
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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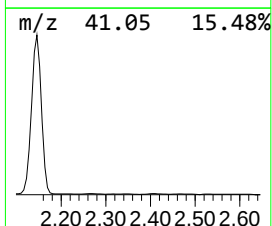
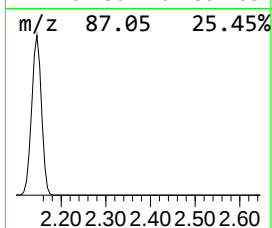
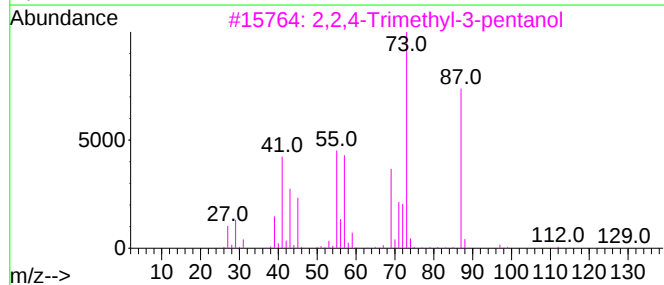
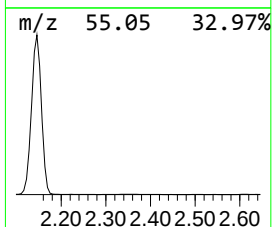
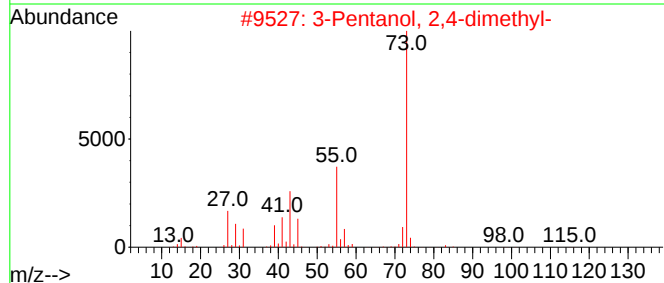
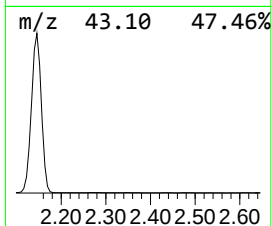
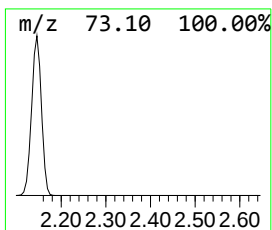
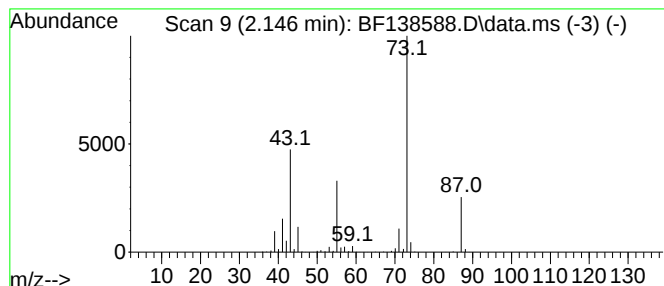
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	82.57 ng	1719230	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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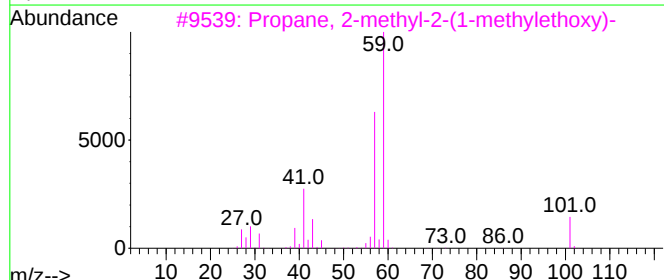
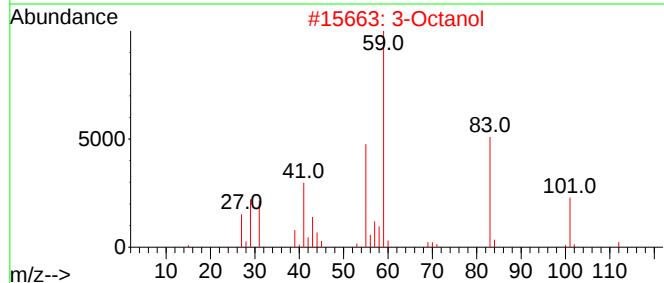
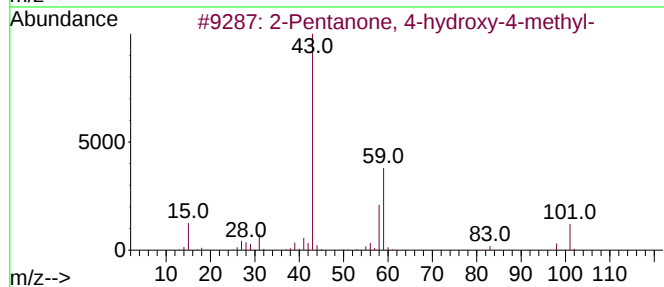
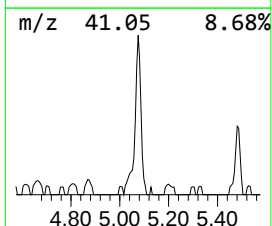
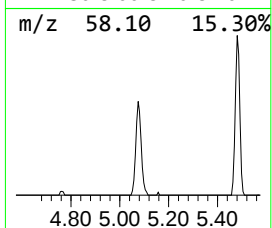
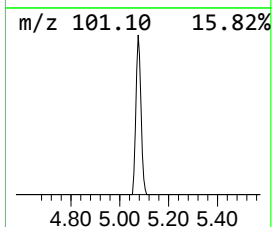
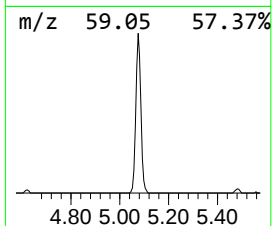
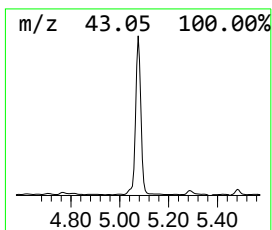
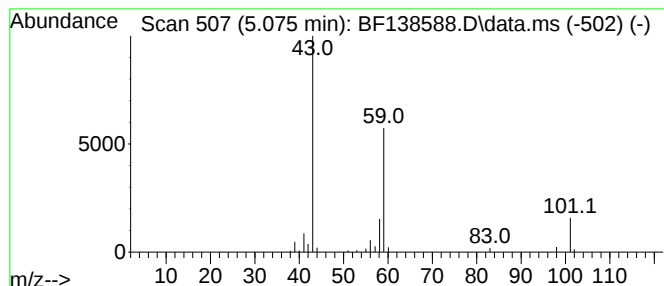
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.46 ng	113600	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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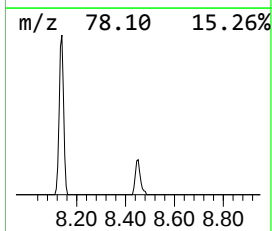
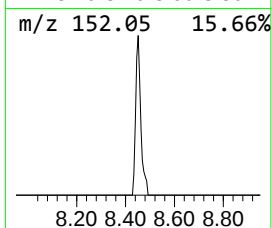
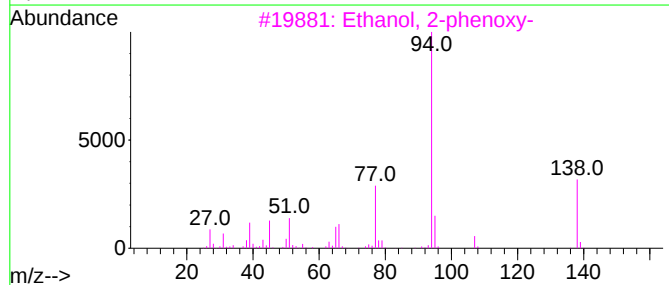
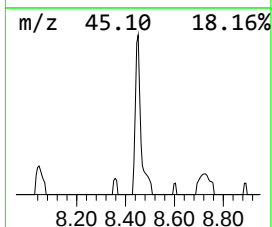
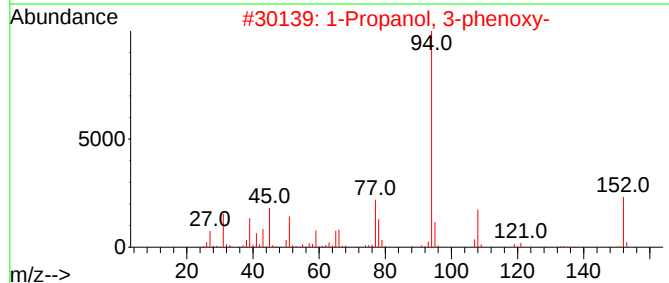
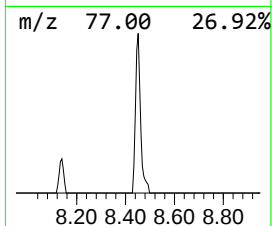
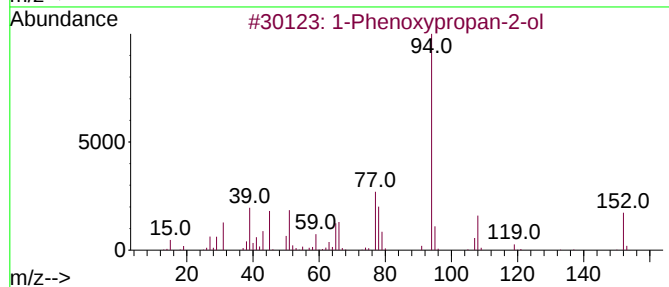
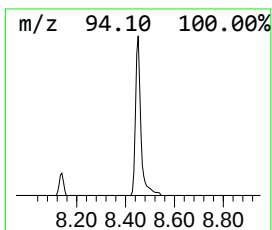
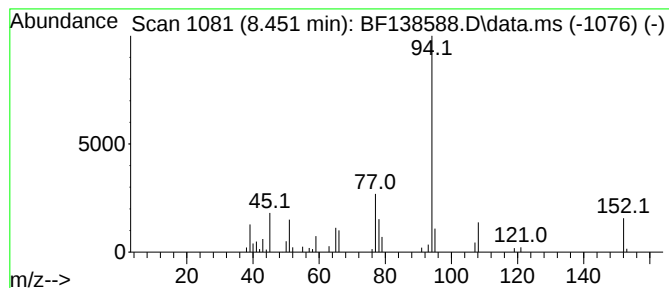
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	2.13 ng	58642	Naphthalene-d8	8.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	74
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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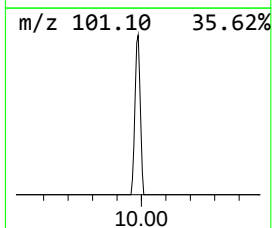
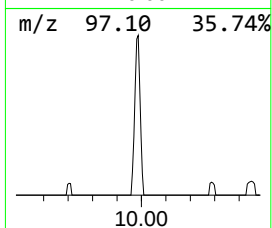
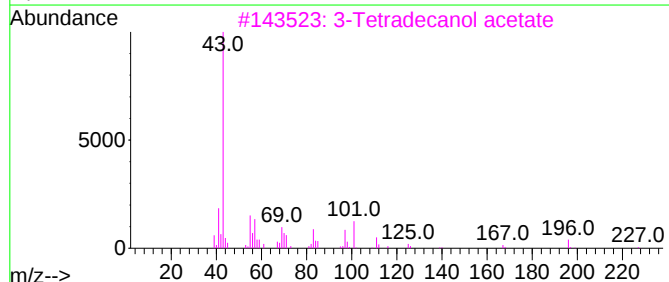
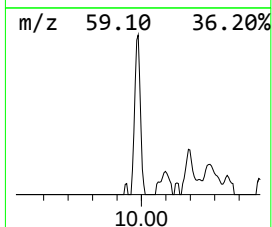
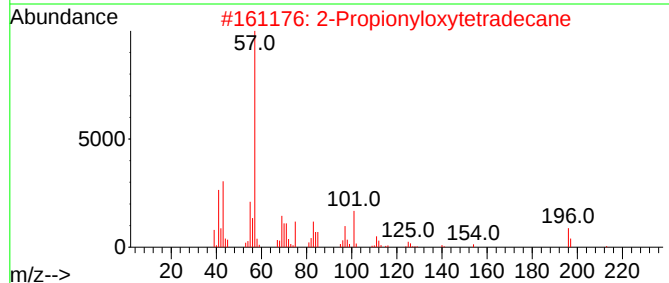
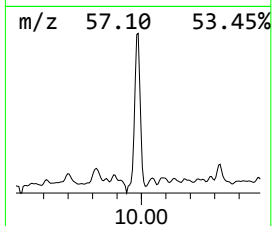
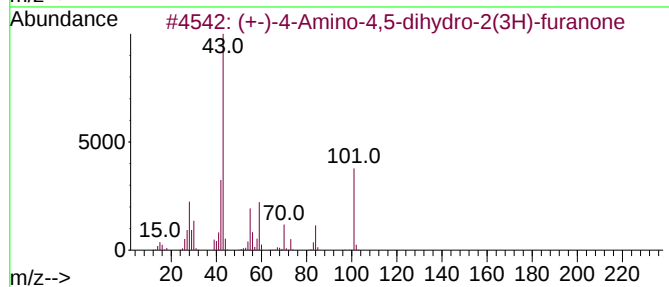
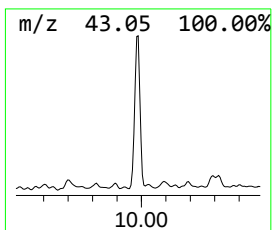
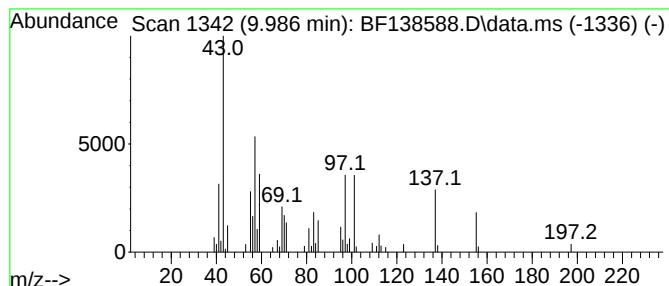
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Peak Number 4 unknown9.986 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	2.00 ng	62164	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	22		
2	2-Propionyloxytetradecane	270	C17H34O2	1000245-62-7	14		
3	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	12		
4	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10		
5	Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	10		



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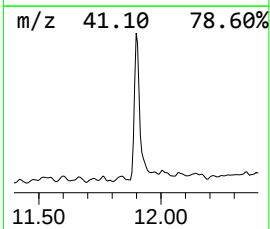
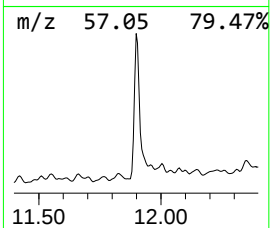
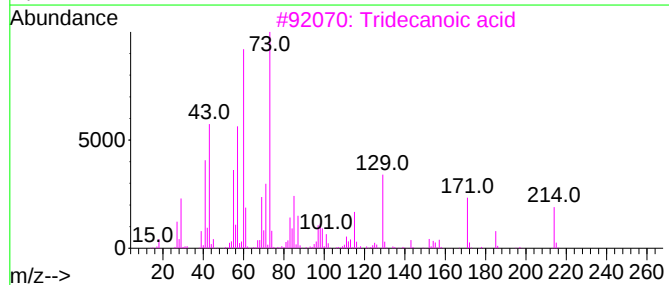
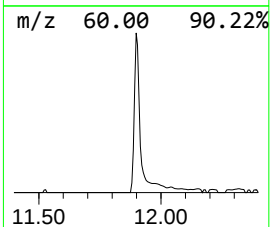
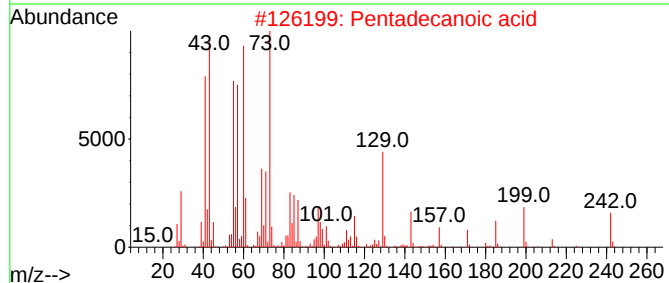
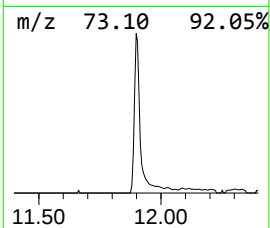
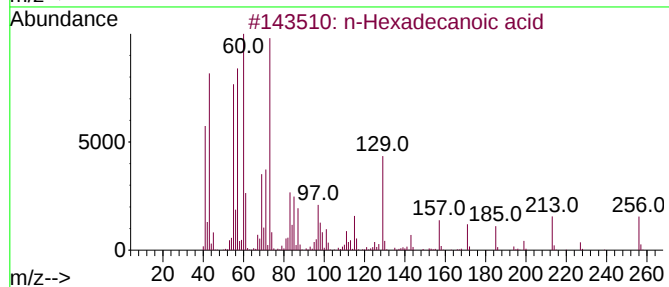
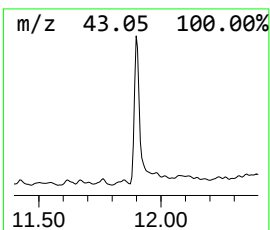
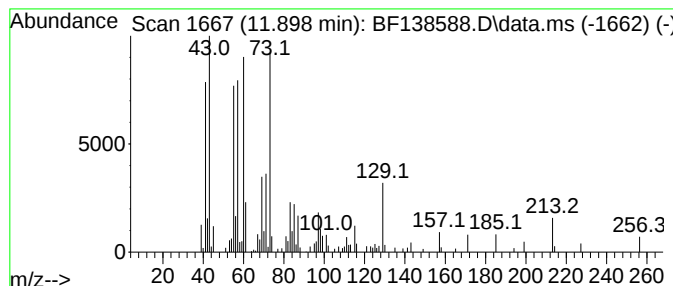
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	5.70 ng	189600	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Undecanoic acid	186	C11H22O2	000112-37-8	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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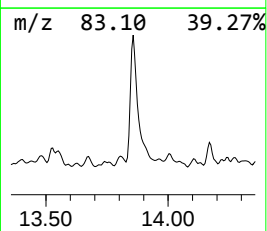
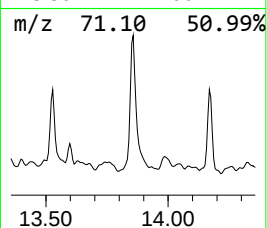
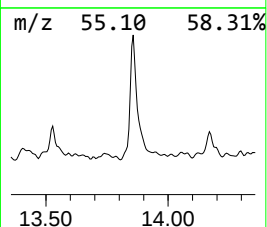
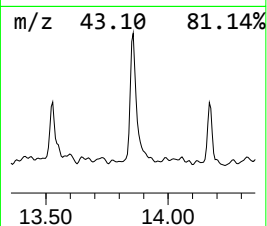
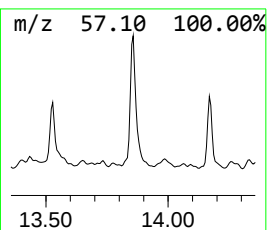
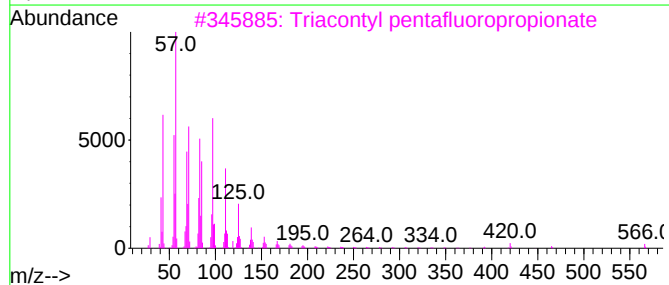
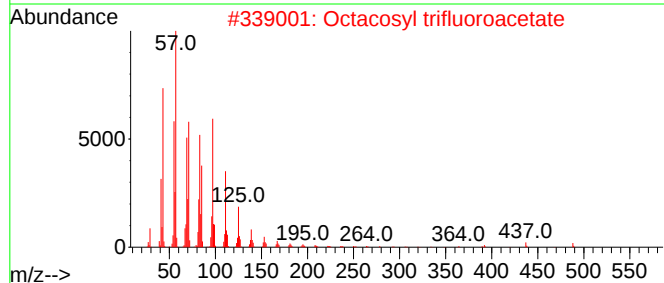
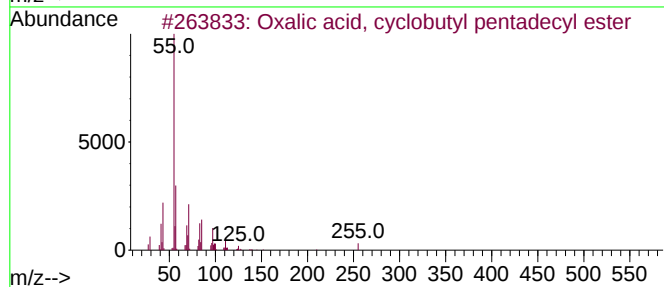
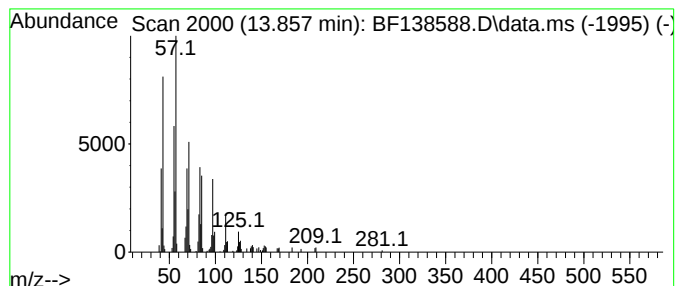
Instrument :
BNA_F
ClientSampleId :
WC-CTW2-BL-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxalic acid, cyclobutyl pen... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	6.28 ng	148724	Chrysene-d12	14.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	91
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
4	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
5	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071924\
Data File : BF138588.D
Acq On : 19 Jul 2024 14:28
Operator : RC/JU
Sample : P3246-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-CTW2-BL-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	82.6	ng	1719230	1	6.857	416447	20.0
2-Pentanone, 4-...	5.075	5.5	ng	113600	1	6.857	416447	20.0
1-Phenoxypropan...	8.451	2.1	ng	58642	2	8.139	550054	20.0
unknown9.986	9.986	2.0	ng	62164	3	9.892	621592	20.0
n-Hexadecanoic ...	11.898	5.7	ng	189600	4	11.374	665098	20.0
Oxalic acid, cy...	13.857	6.3	ng	148724	5	14.010	473905	20.0