

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071924\
 Data File : BF138592.D
 Acq On : 19 Jul 2024 16:30
 Operator : RC/JU
 Sample : P3246-21
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-CTW2-BL-05

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: BF138592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	3	12	19	rVB	1743916	2764735	100.00%	13.394%
2	3.393	215	221	240	rBV	70838	167984	6.08%	0.814%
3	5.087	504	509	520	rVB	130236	196986	7.12%	0.954%
4	5.487	571	577	582	rBV	1798604	2364973	85.54%	11.457%
5	6.492	742	748	764	rBV	1807557	2535387	91.70%	12.282%
6	6.686	776	781	786	rBV	24764	31666	1.15%	0.153%
7	6.857	805	810	815	rBV	368183	442776	16.02%	2.145%
8	7.422	899	906	911	rBV	1138244	1567568	56.70%	7.594%
9	8.139	1022	1028	1033	rBV	469617	585950	21.19%	2.839%
10	8.451	1076	1081	1093	rBV	40899	63767	2.31%	0.309%
11	9.216	1204	1211	1216	rBV	1893107	2488977	90.03%	12.058%
12	9.892	1320	1326	1331	rBV	535751	660942	23.91%	3.202%
13	9.986	1336	1342	1349	rBV	70296	110106	3.98%	0.533%
14	10.680	1454	1460	1475	rBV	1318677	1739687	62.92%	8.428%
15	11.374	1573	1578	1585	rBV	560715	709191	25.65%	3.436%
16	11.898	1662	1667	1681	rBV2	132593	226360	8.19%	1.097%
17	12.686	1796	1801	1813	rBV	25645	48705	1.76%	0.236%
18	12.963	1842	1848	1853	rBV	1873942	2415272	87.36%	11.701%
19	13.633	1957	1962	1970	rVB	184838	241315	8.73%	1.169%
20	13.857	1994	2000	2015	rBV	112962	232727	8.42%	1.127%
21	14.010	2021	2026	2039	rVB	345120	457908	16.56%	2.218%
22	14.480	2101	2106	2120	rBV3	21177	69793	2.52%	0.338%
23	15.115	2210	2214	2219	rBV	19265	28328	1.02%	0.137%
24	15.474	2270	2275	2287	rVB	278953	447636	16.19%	2.169%
25	15.998	2359	2364	2371	rBV8	13880	43604	1.58%	0.211%

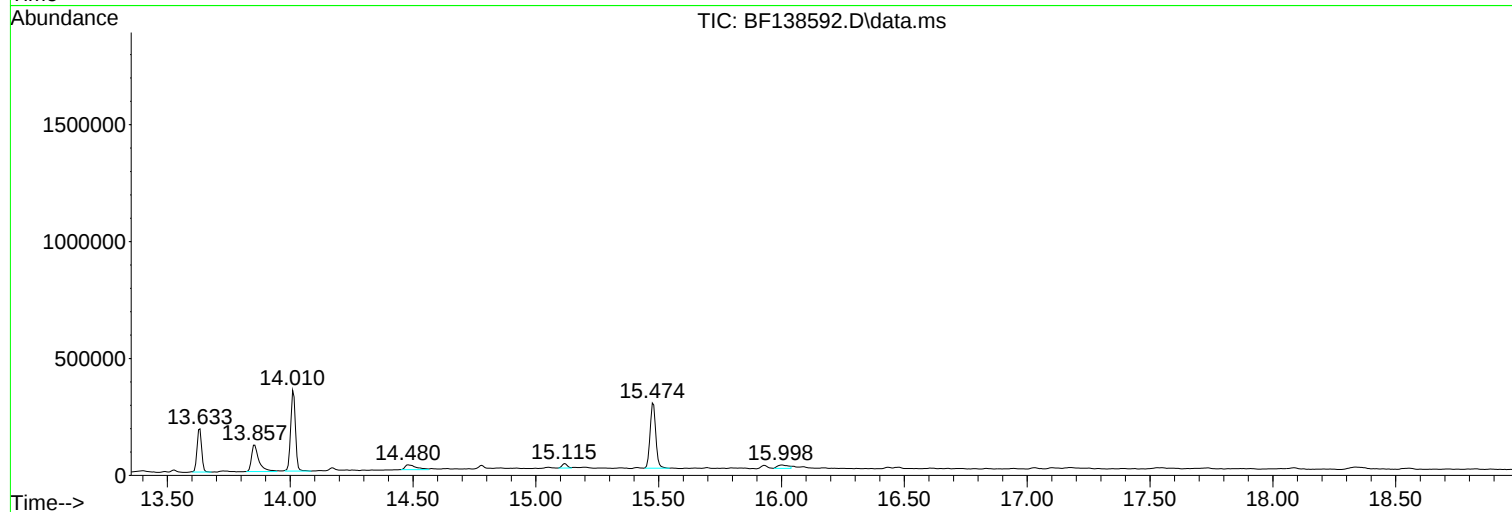
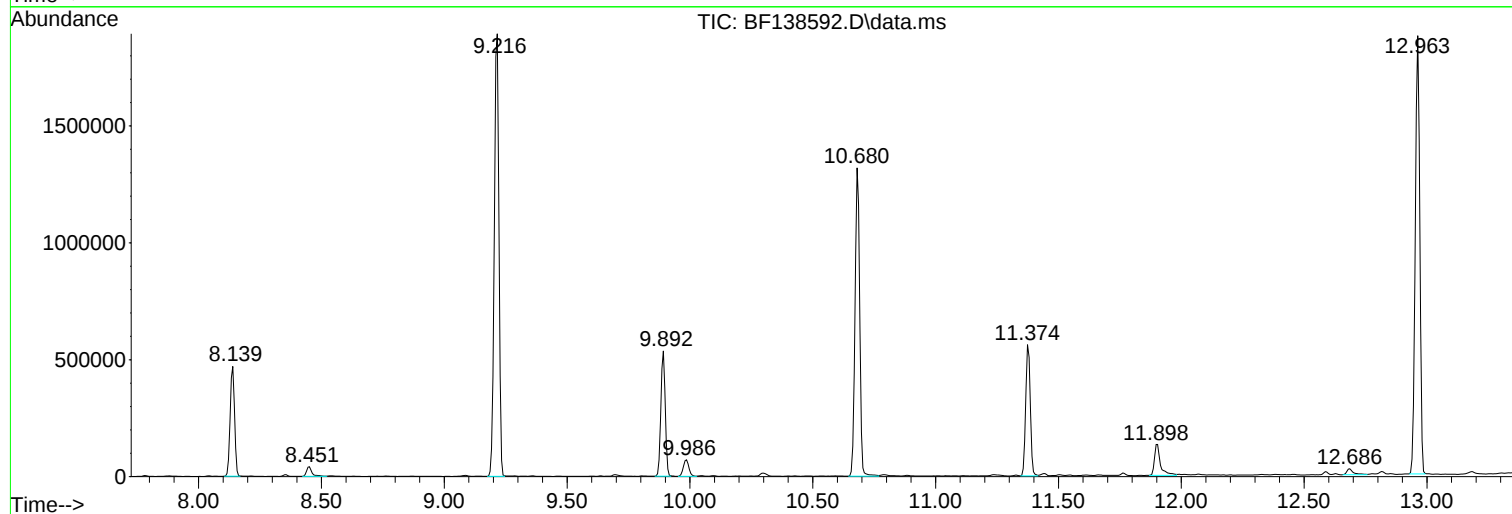
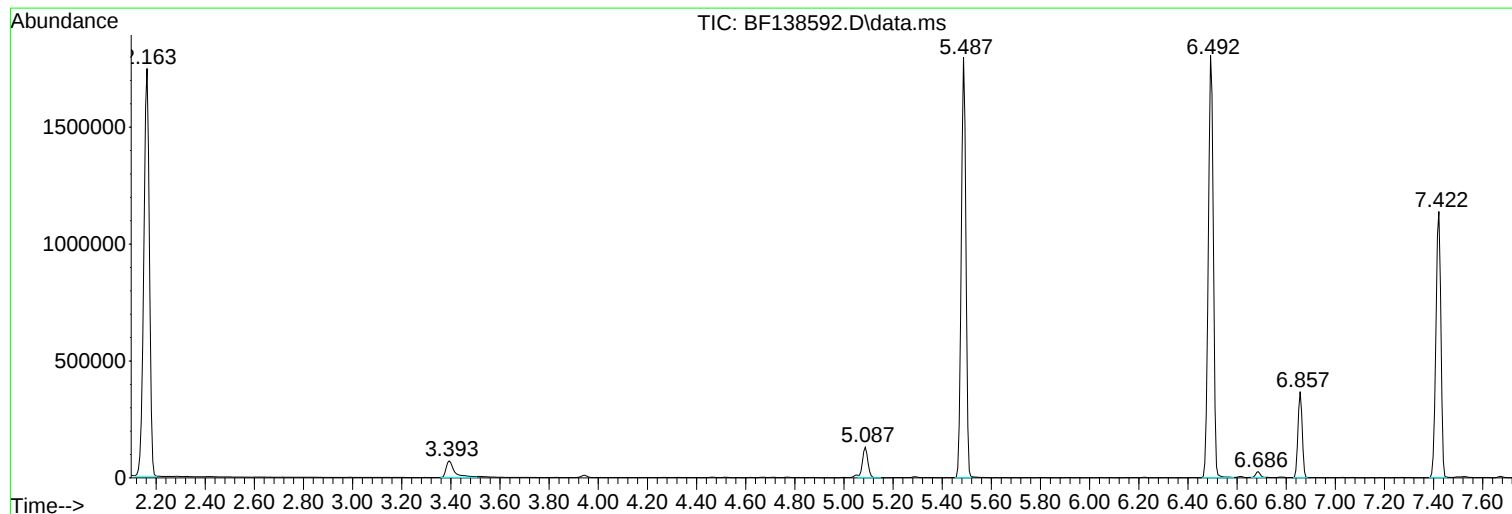
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-CTW2-BL-05

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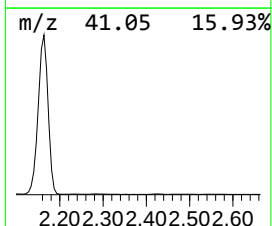
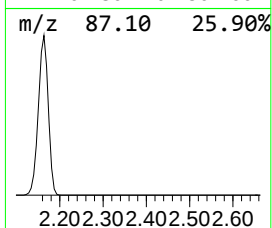
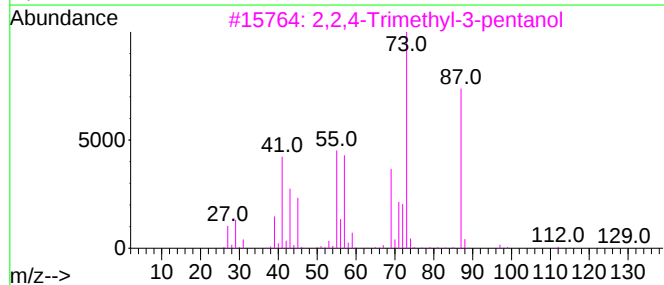
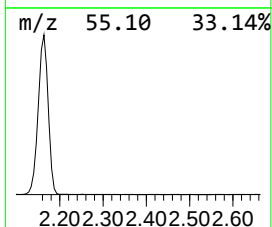
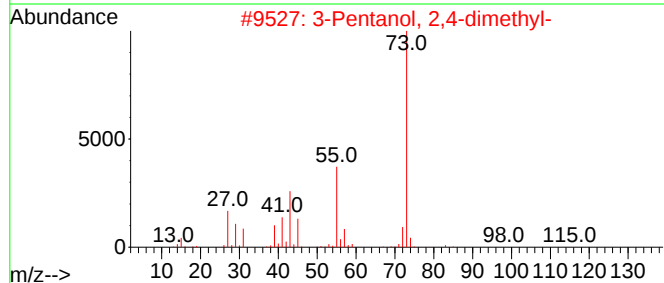
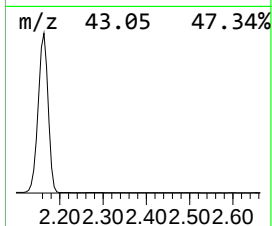
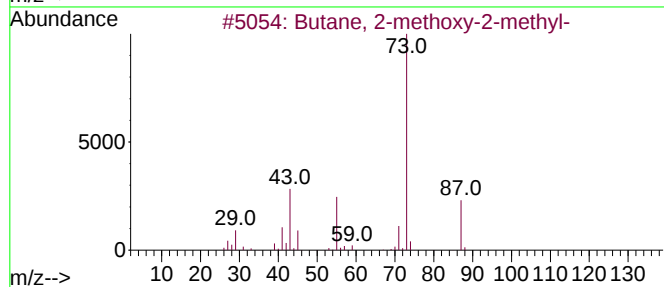
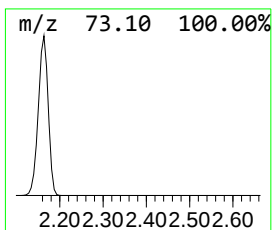
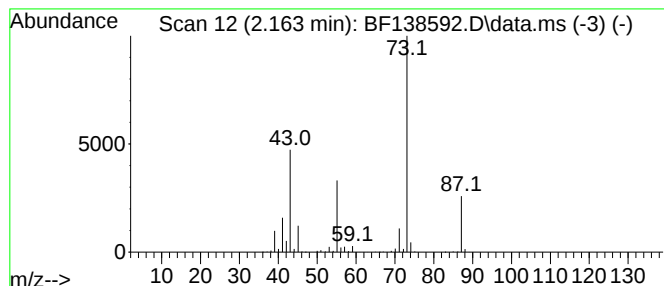
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	124.88 ng	2764740	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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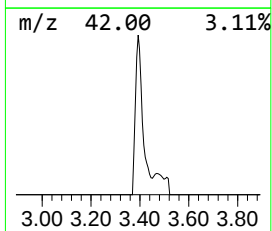
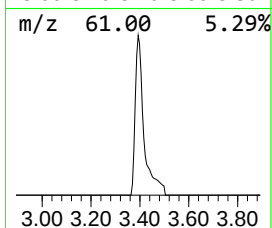
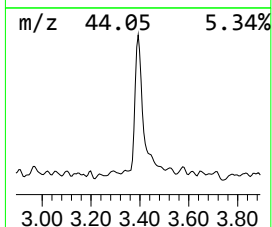
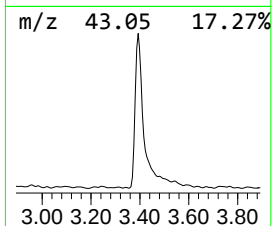
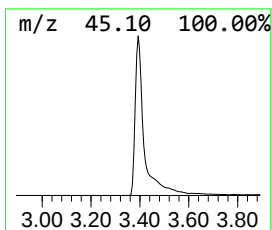
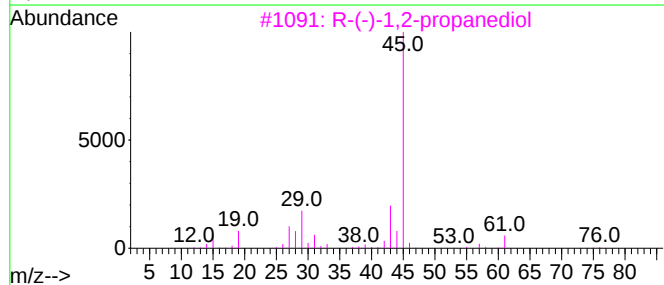
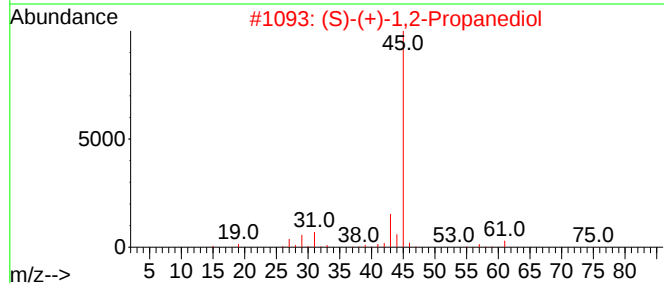
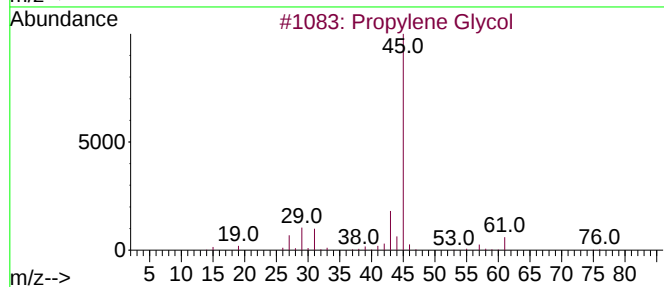
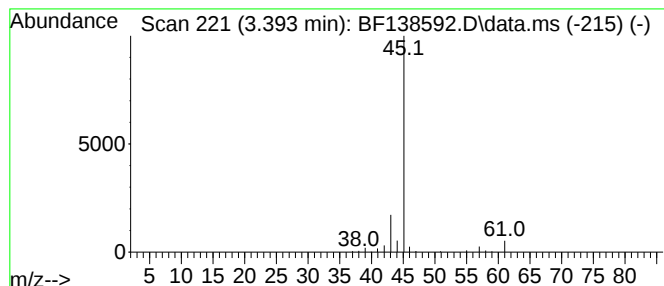
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	7.59 ng	167984	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	74
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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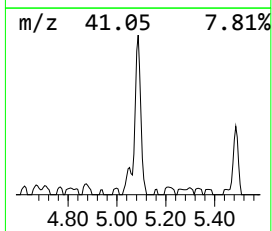
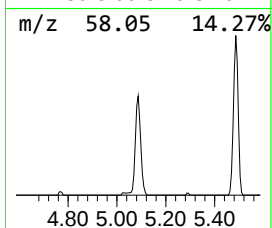
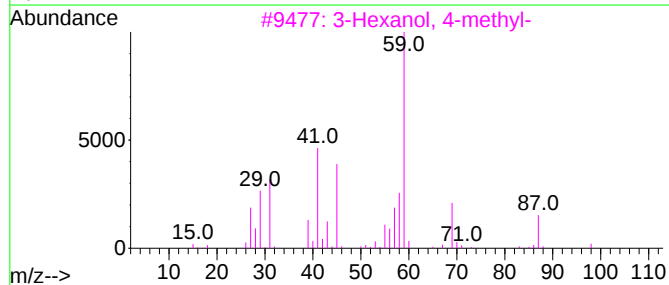
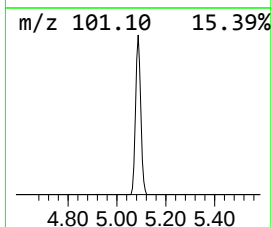
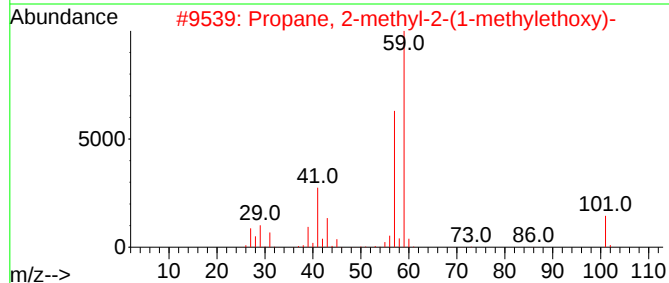
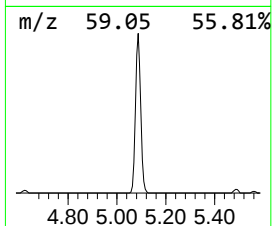
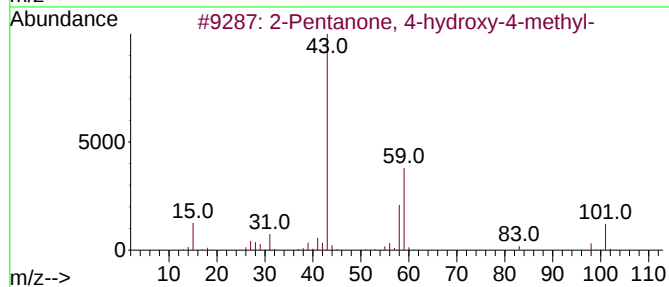
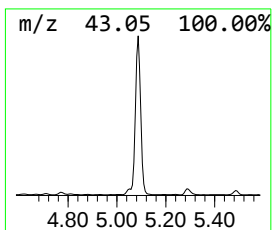
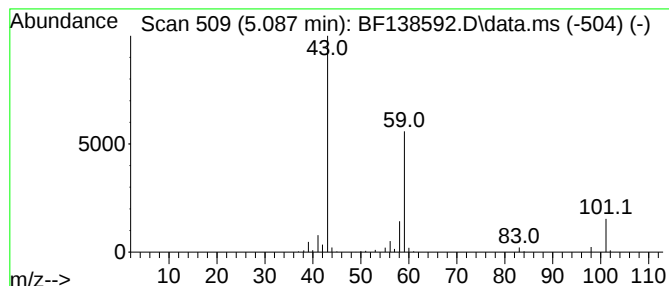
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	8.90 ng	196986	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		



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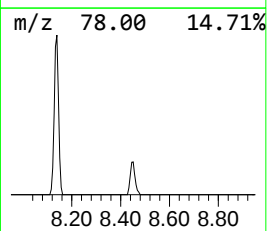
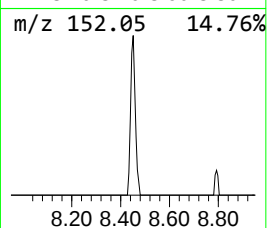
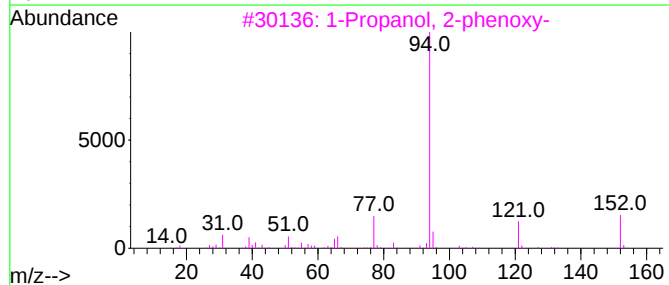
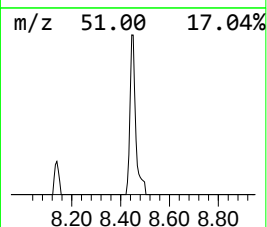
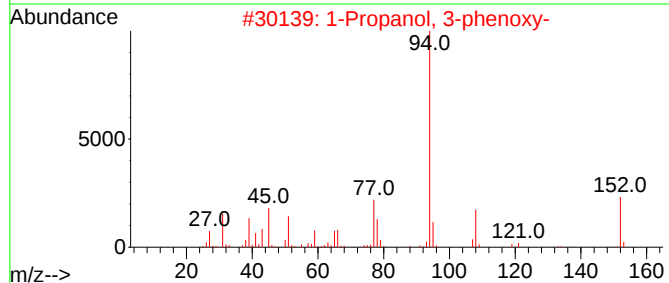
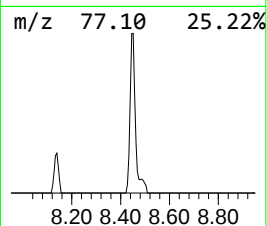
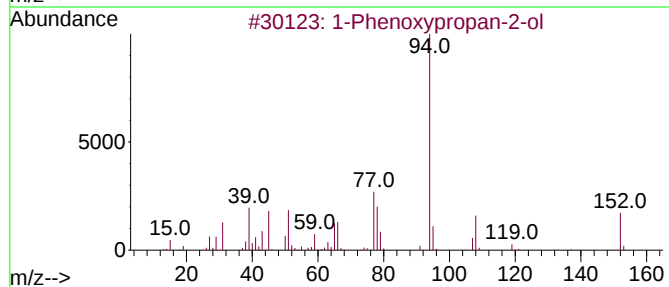
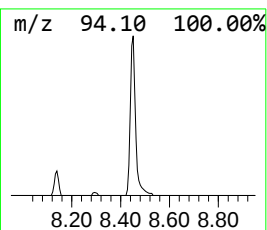
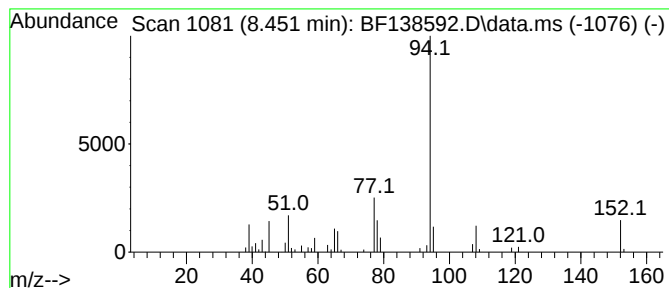
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	2.18 ng	63767	Naphthalene-d8	8.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
5			Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53



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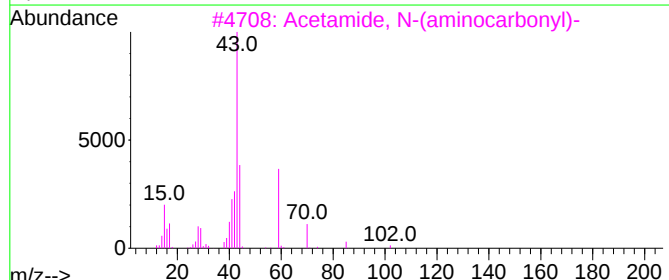
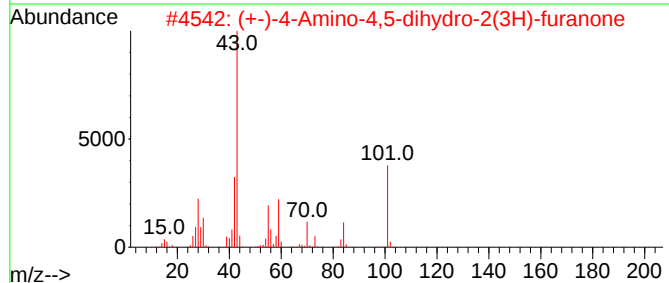
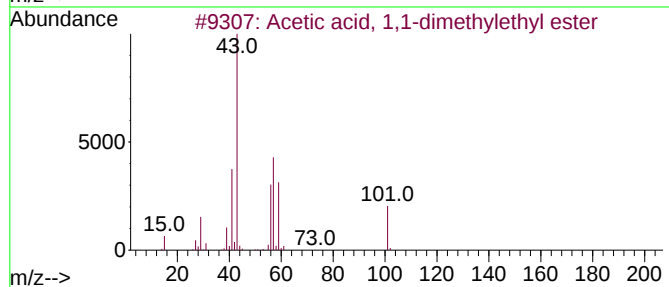
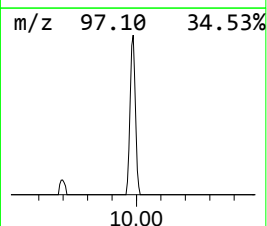
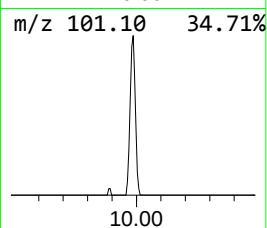
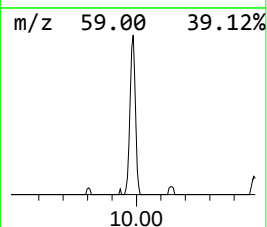
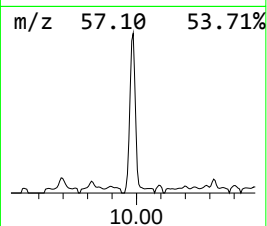
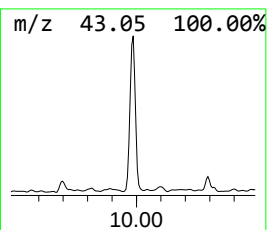
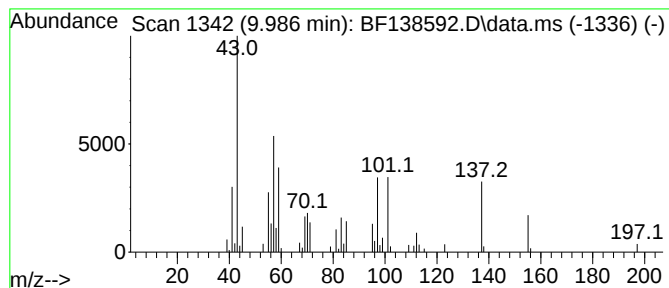
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown9.986 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	3.33 ng	110106	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	27
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	27
3			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	14
4			5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	12
5			4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	10



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WC-CTW2-BL-05

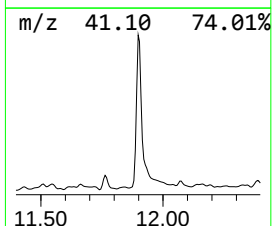
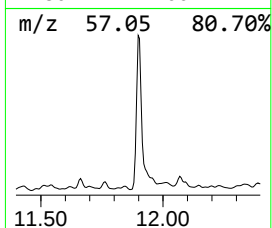
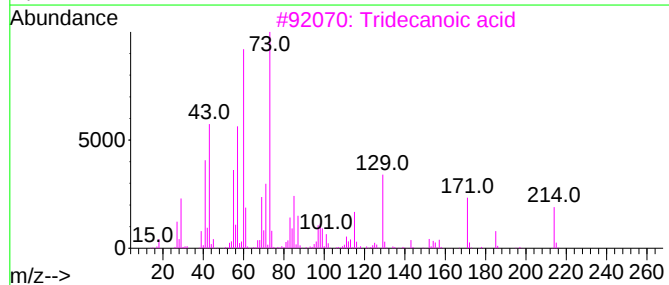
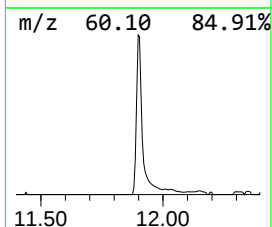
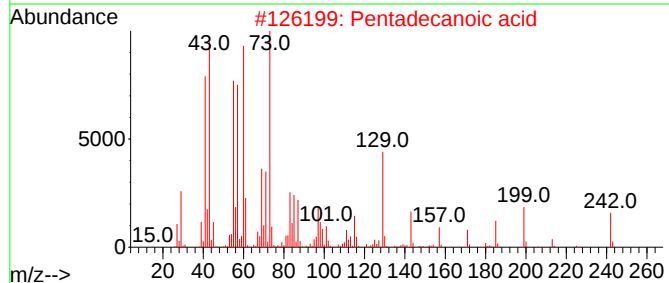
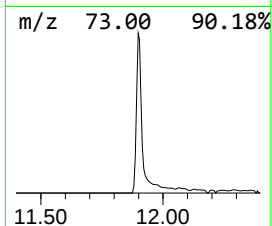
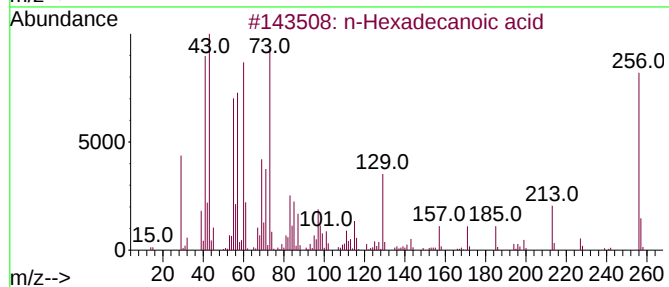
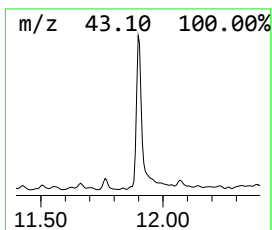
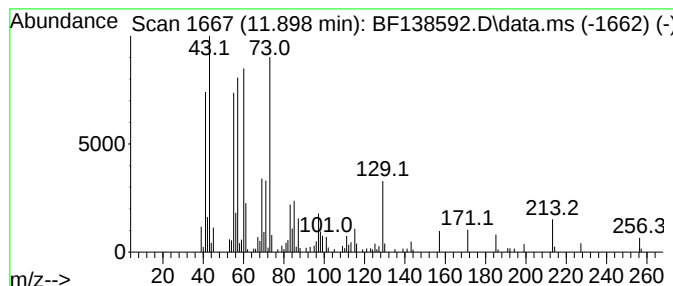
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	6.38 ng	226360	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	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071924\
Data File : BF138592.D
Acq On : 19 Jul 2024 16:30
Operator : RC/JU
Sample : P3246-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-CTW2-BL-05

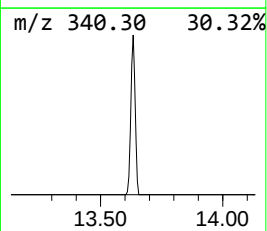
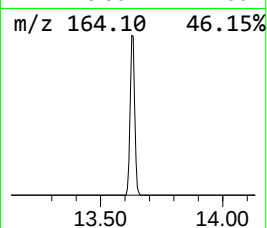
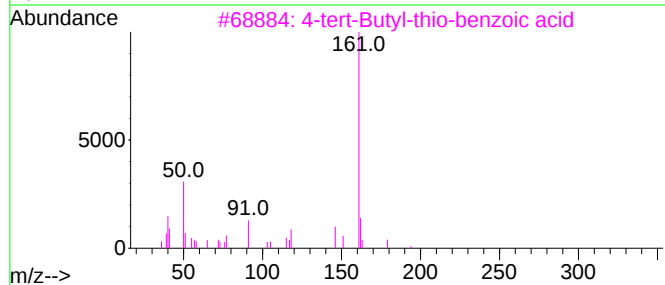
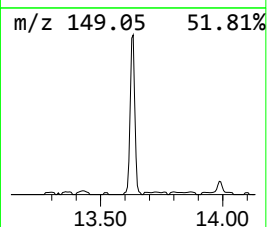
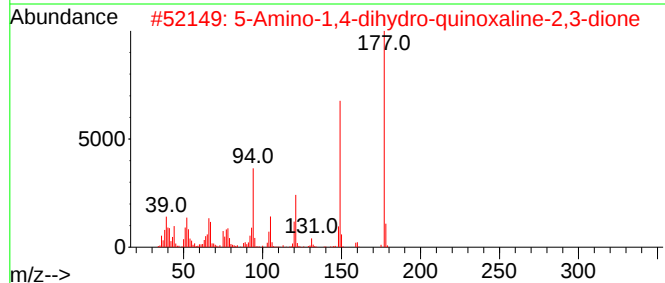
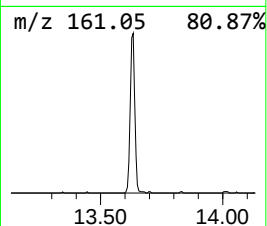
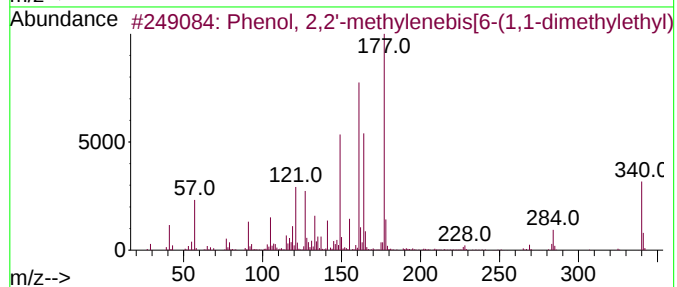
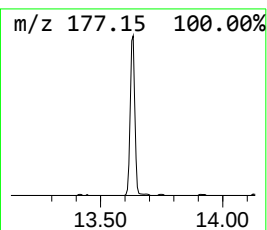
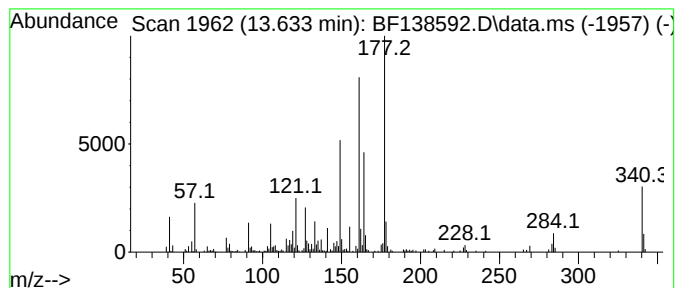
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 2,2'-methylenebis[6... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.633	10.54 ng	241315	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,2'-methylenebis[6-(1,1...	340	C23H32O2	000119-47-1	99
2			5-Amino-1,4-dihydro-quinoxaline-...	177	C8H7N3O2	076097-87-5	30
3			4-tert-Butyl-thio-benzoic acid	194	C11H14OS	072207-52-4	20
4			5-Methyl-2,4-diisopropylphenol	192	C13H20O	040625-96-5	18
5			Benzoic acid, 4-butyl-, 4-methox...	284	C18H20O3	035684-23-2	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071924\
Data File : BF138592.D
Acq On : 19 Jul 2024 16:30
Operator : RC/JU
Sample : P3246-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-CTW2-BL-05

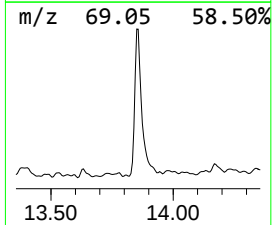
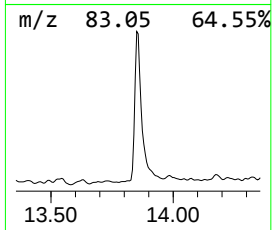
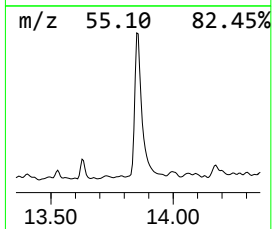
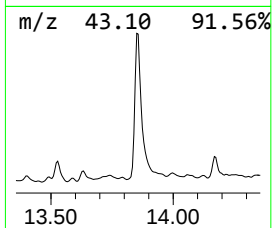
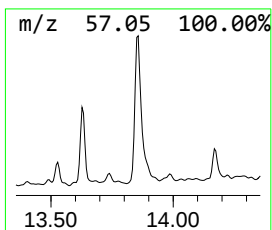
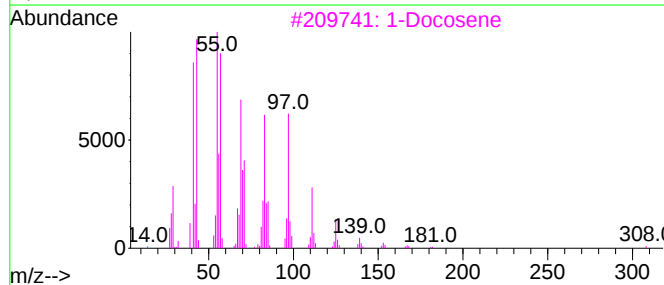
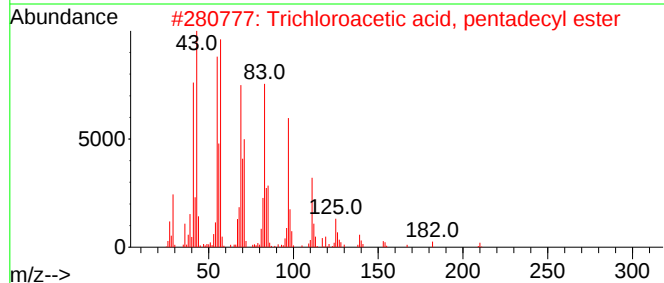
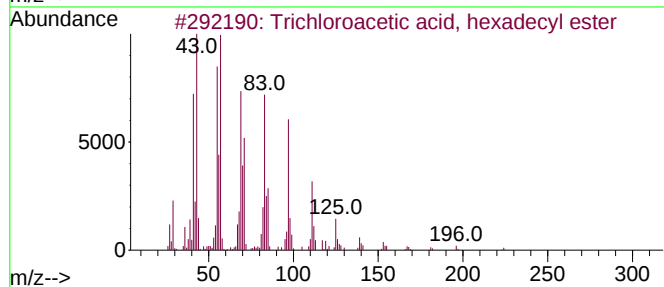
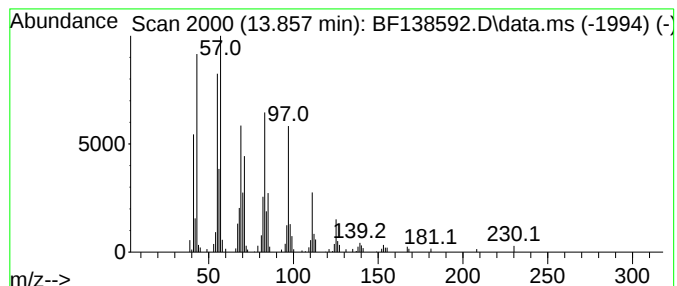
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	10.16 ng	232727	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
3			1-Docosene	308	C22H44	001599-67-3	95
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071924\
Data File : BF138592.D
Acq On : 19 Jul 2024 16:30
Operator : RC/JU
Sample : P3246-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

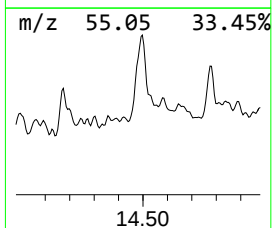
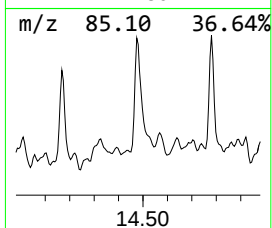
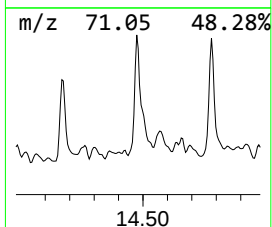
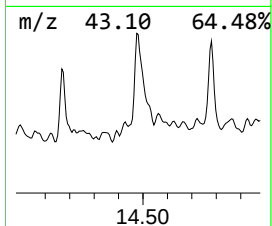
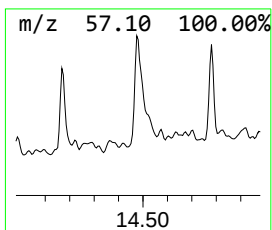
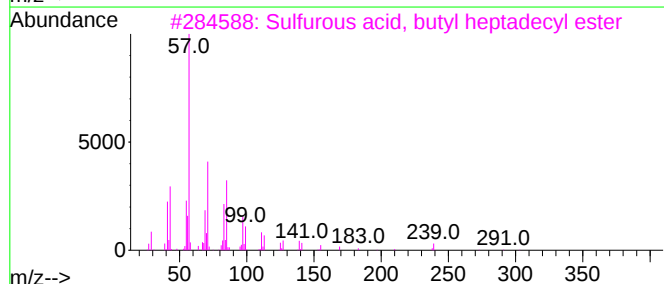
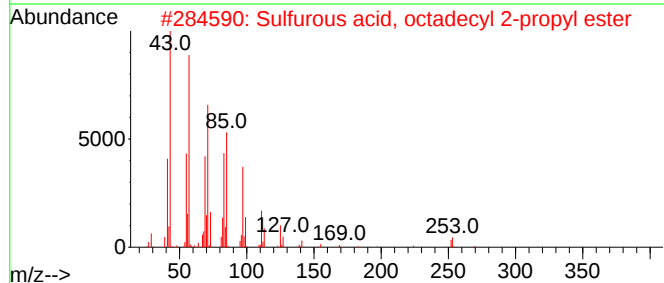
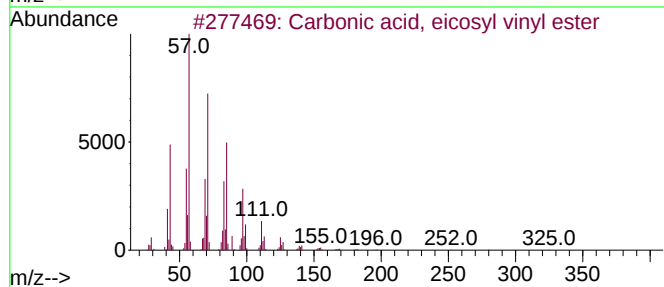
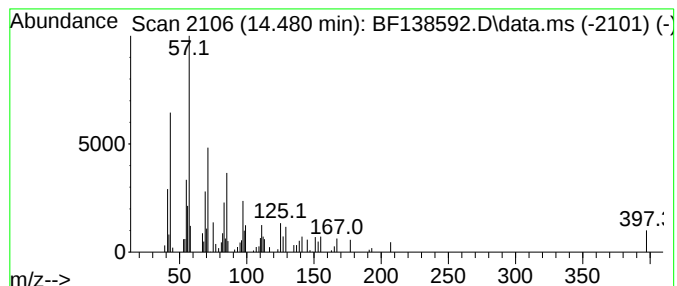
Instrument :
BNA_F
ClientSampleId :
WC-CTW2-BL-05

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 9 Carbonic acid, eicosyl vinyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.480	3.05 ng	69793	Chrysene-d12	14.009	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	83
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	74
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	72
4	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	72
5	Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071924\
Data File : BF138592.D
Acq On : 19 Jul 2024 16:30
Operator : RC/JU
Sample : P3246-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-CTW2-BL-05

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.163	124.9	ng	2764740	1	6.857	442776	20.0
Propylene Glycol	3.393	7.6	ng	167984	1	6.857	442776	20.0
2-Pentanone, 4-...	5.087	8.9	ng	196986	1	6.857	442776	20.0
1-Phenoxypropan...	8.451	2.2	ng	63767	2	8.139	585950	20.0
unknown9.986	9.986	3.3	ng	110106	3	9.892	660942	20.0
n-Hexadecanoic ...	11.898	6.4	ng	226360	4	11.374	709191	20.0
Phenol, 2,2'-me...	13.633	10.5	ng	241315	5	14.009	457908	20.0
Trichloroacetic...	13.857	10.2	ng	232727	5	14.009	457908	20.0
Carbonic acid, ...	14.480	3.0	ng	69793	5	14.009	457908	20.0