

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
 Data File : BF139185.D
 Acq On : 27 Aug 2024 14:17
 Operator : RC/JU
 Sample : P3717-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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-BF082724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139185.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	15	22	rVB	1292435	1993936	100.00%	13.289%
2	3.381	213	219	246	rBV	20669	59679	2.99%	0.398%
3	5.104	503	512	521	rBV	69399	108261	5.43%	0.722%
4	5.504	574	580	585	rBV	1262255	1643053	82.40%	10.951%
5	6.510	745	751	756	rBV	1263690	1690337	84.77%	11.266%
6	6.893	811	816	821	rBV	395395	484333	24.29%	3.228%
7	7.451	905	911	916	rBV	807029	1017852	51.05%	6.784%
8	7.704	950	954	958	rVB	38170	43913	2.20%	0.293%
9	8.175	1028	1034	1039	rBV	480014	602292	30.21%	4.014%
10	8.481	1082	1086	1097	rVB	66438	82505	4.14%	0.550%
11	9.245	1211	1216	1221	rBV	1532866	1858839	93.22%	12.389%
12	9.922	1326	1331	1336	rBV	526973	663295	33.27%	4.421%
13	10.016	1342	1347	1356	rBV	27612	41937	2.10%	0.280%
14	10.710	1460	1465	1470	rBV	833047	1016576	50.98%	6.775%
15	11.410	1579	1584	1591	rVB	483002	589314	29.56%	3.928%
16	11.939	1668	1674	1685	rBV	190861	283143	14.20%	1.887%
17	12.622	1785	1790	1801	rBV	24219	50257	2.52%	0.335%
18	12.722	1802	1807	1820	rBV	80584	127390	6.39%	0.849%
19	12.851	1825	1829	1833	rVV	17162	27185	1.36%	0.181%
20	12.992	1848	1853	1859	rBV	1158497	1494513	74.95%	9.961%
21	13.598	1946	1956	1960	rBV10	7961	26893	1.35%	0.179%
22	13.898	2002	2007	2020	rBV	57182	124754	6.26%	0.831%
23	14.045	2027	2032	2043	rVB	384418	507664	25.46%	3.384%
24	14.910	2176	2179	2185	rVB	14420	20705	1.04%	0.138%
25	15.086	2206	2209	2219	rVB	11214	25662	1.29%	0.171%
26	15.180	2221	2225	2229	rBV2	15211	22318	1.12%	0.149%
27	15.521	2277	2283	2288	rBV	246031	372537	18.68%	2.483%
28	16.015	2362	2367	2371	rBV3	13517	24824	1.24%	0.165%

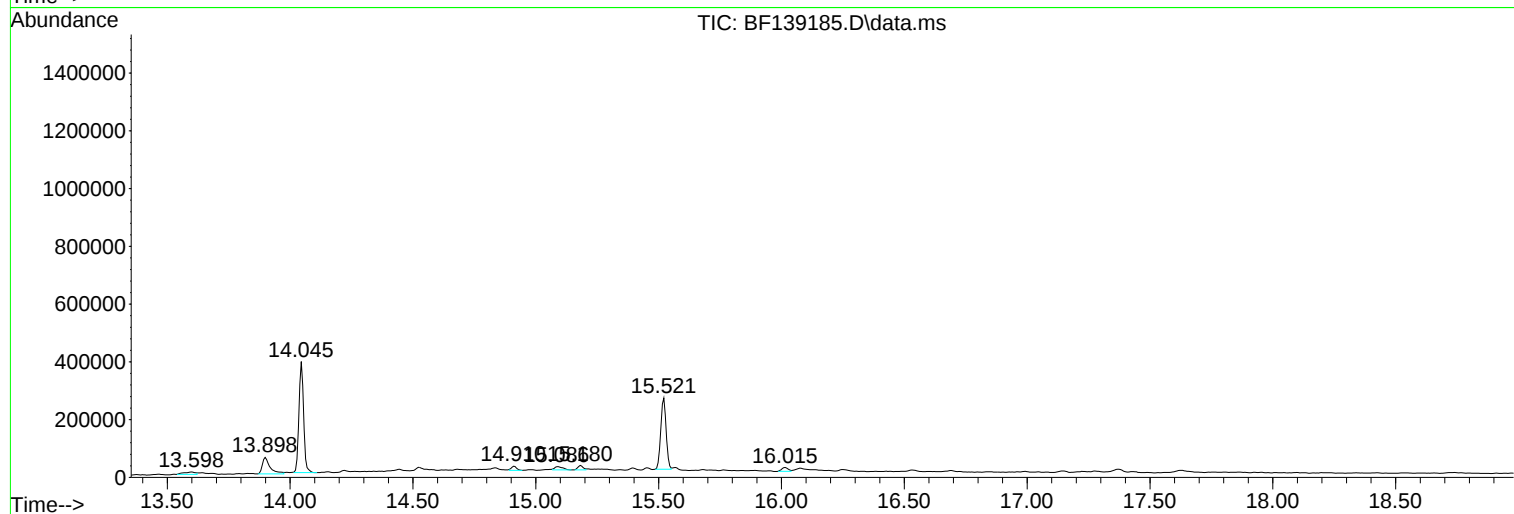
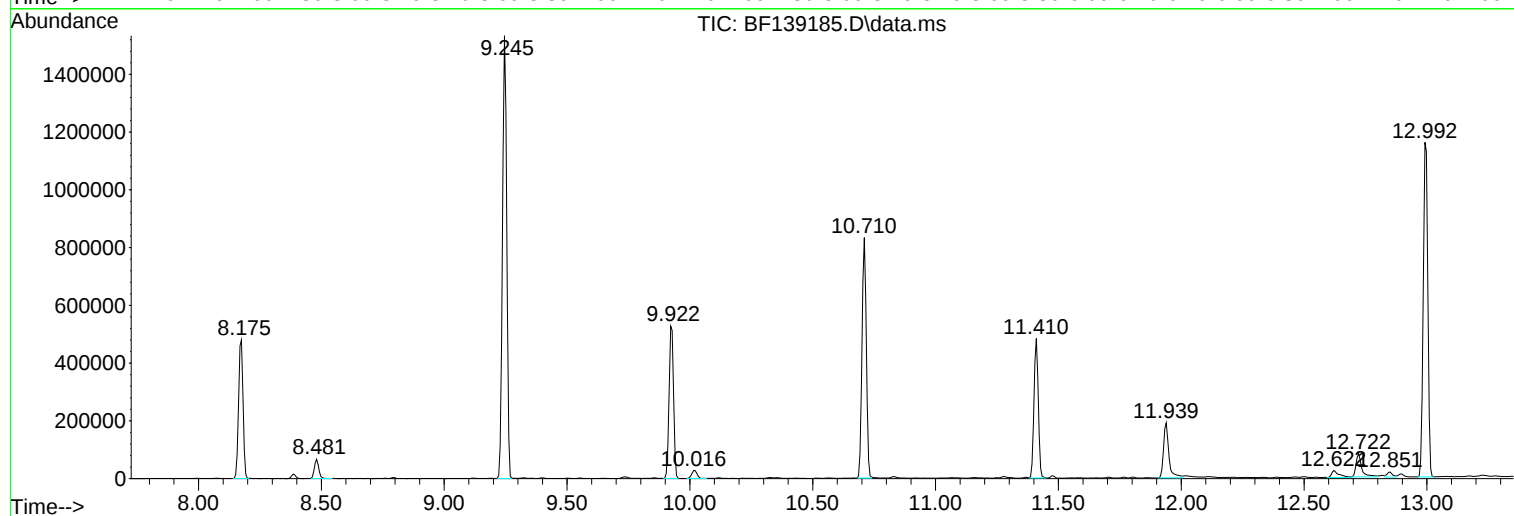
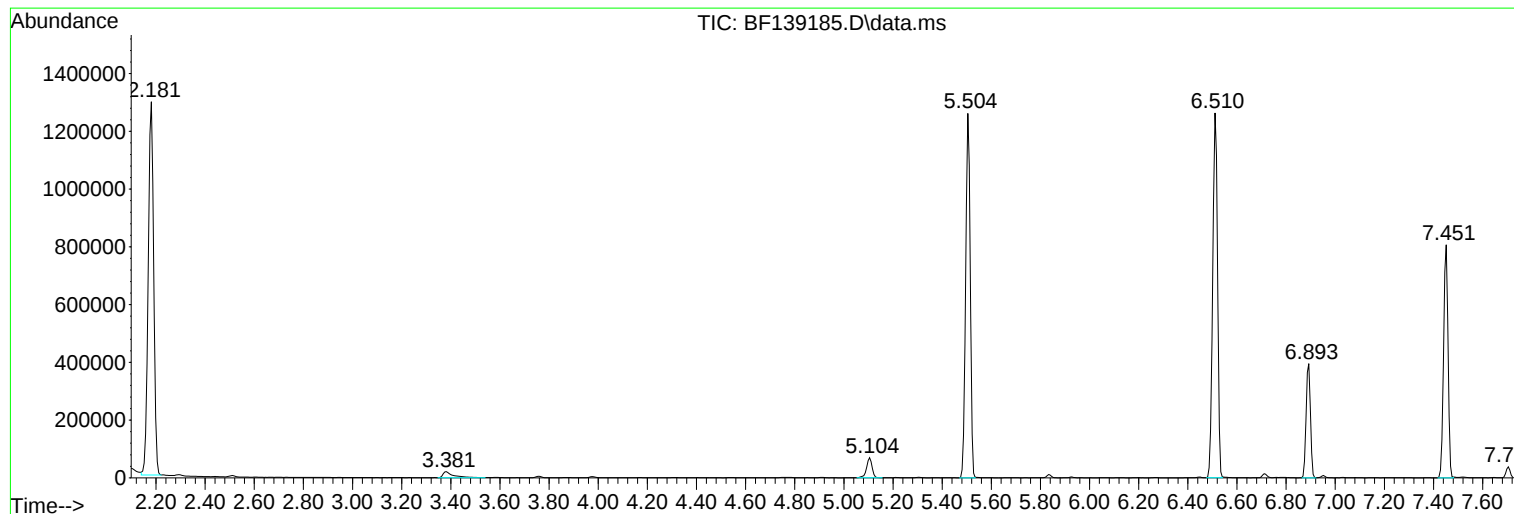
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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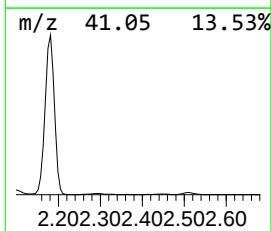
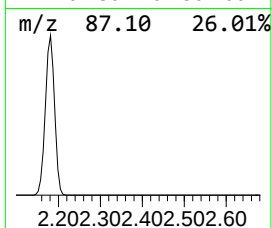
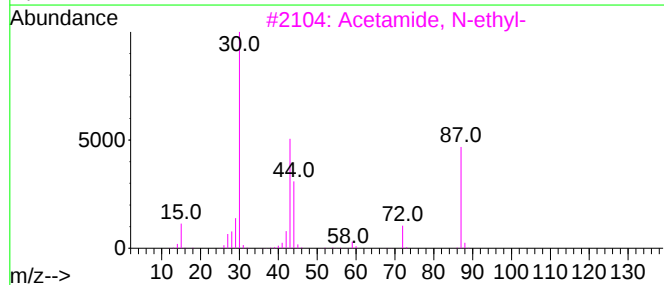
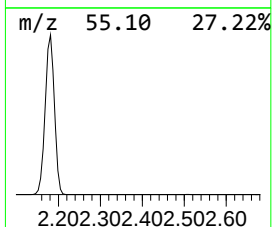
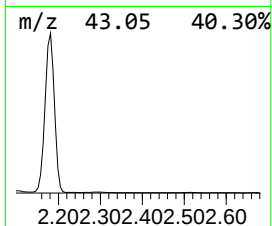
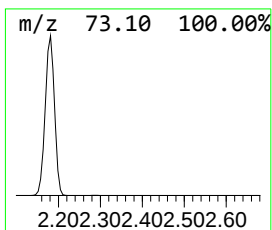
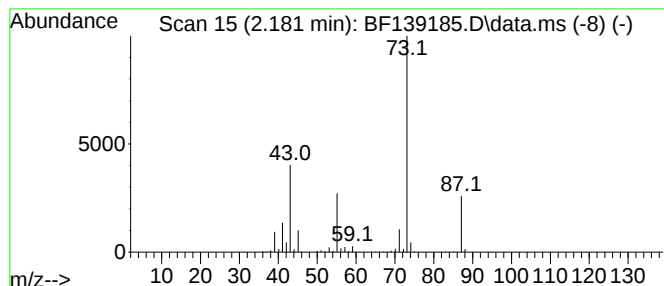
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	82.34 ng	1993940	1,4-Dichlorobenzene-d4	6.893

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	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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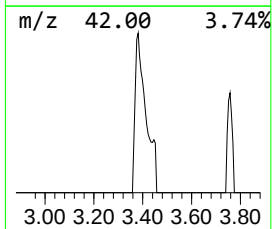
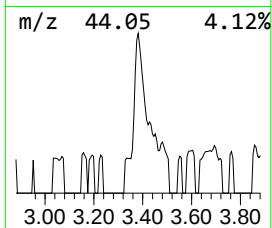
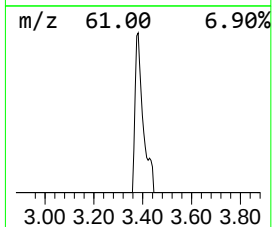
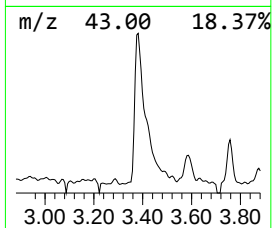
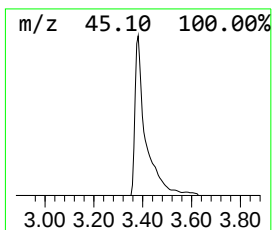
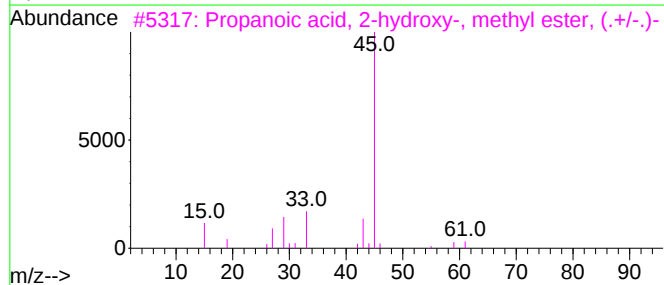
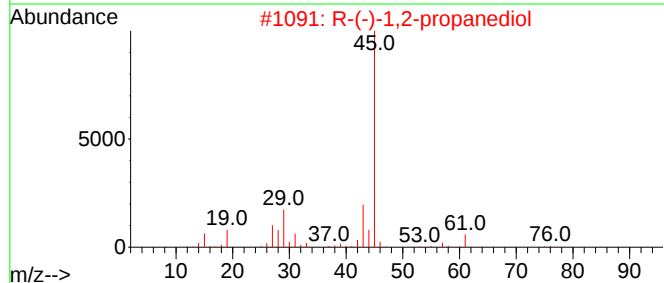
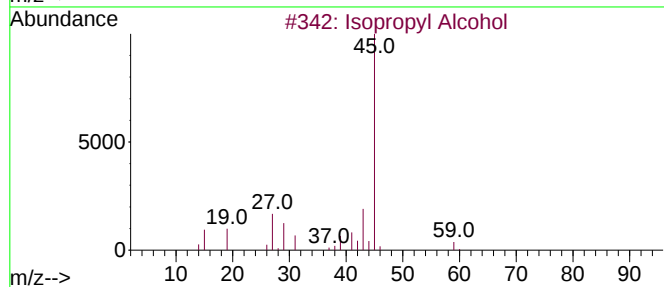
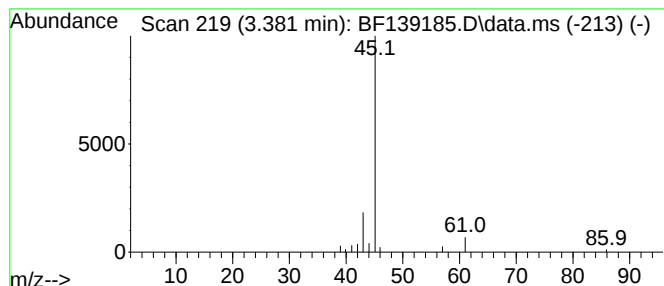
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Peak Number 2 unknown3.381 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.381	2.46 ng	59679	1,4-Dichlorobenzene-d4	6.893

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



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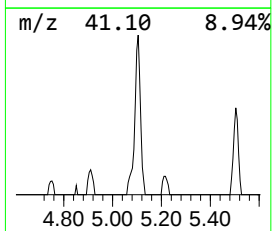
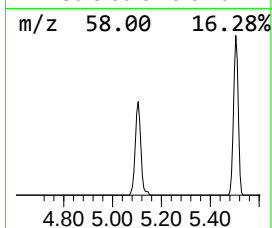
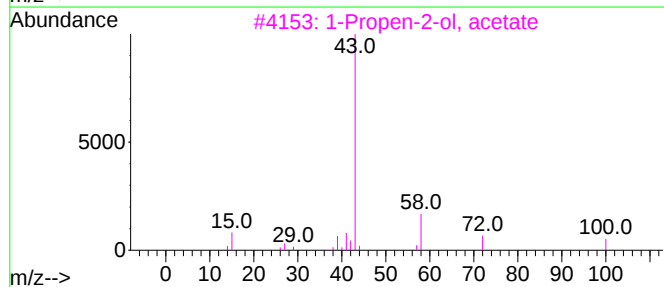
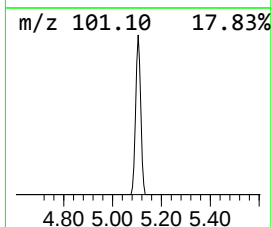
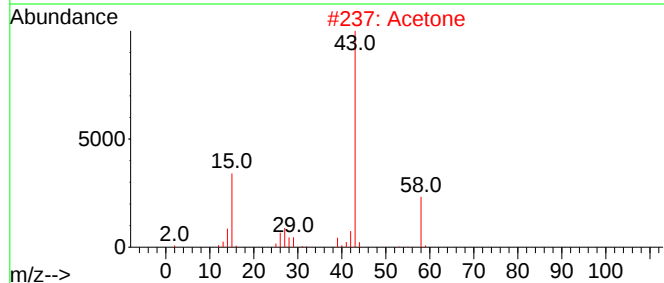
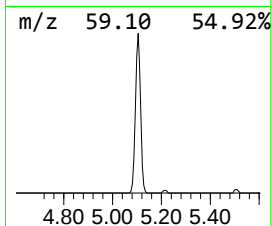
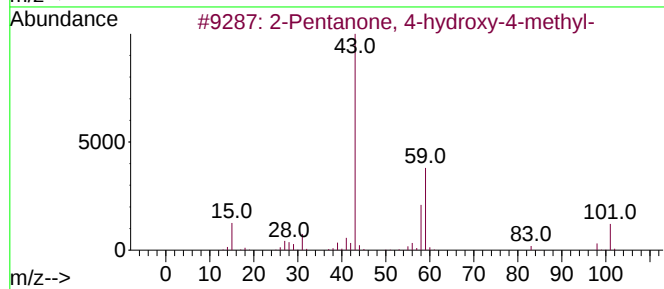
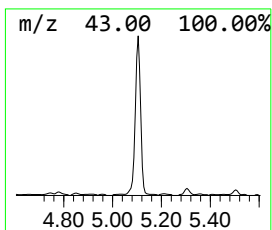
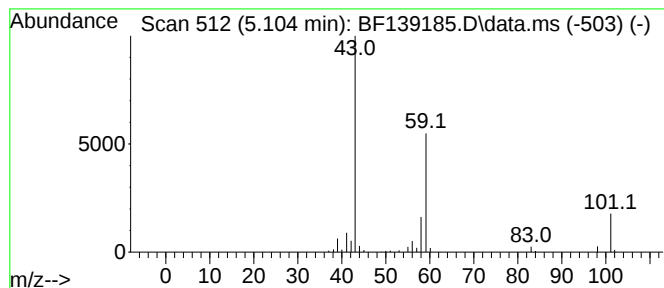
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	4.47 ng	108261	1,4-Dichlorobenzene-d4	6.893

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetone	58	C3H6O	000067-64-1	12
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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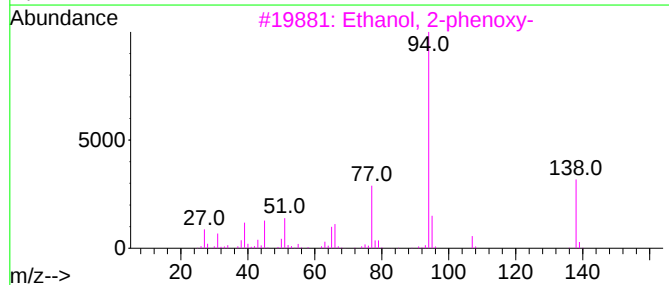
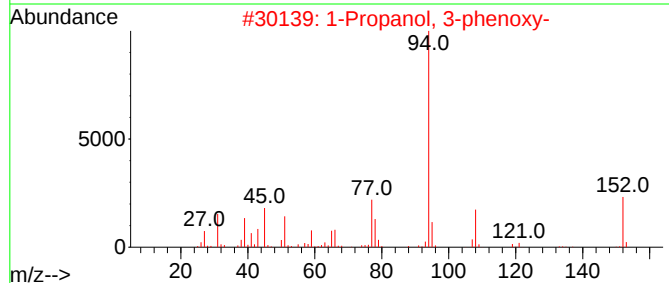
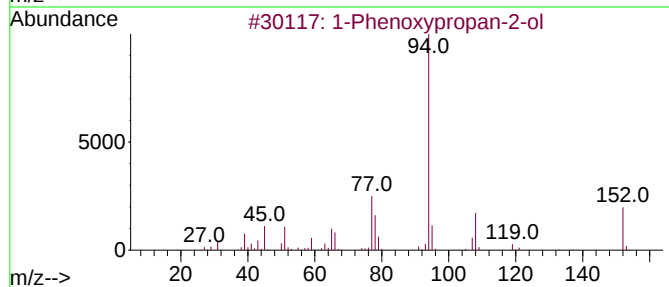
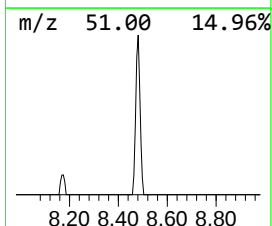
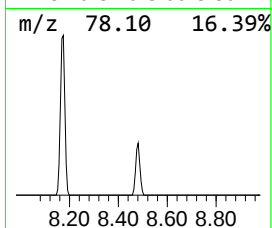
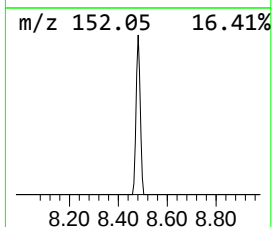
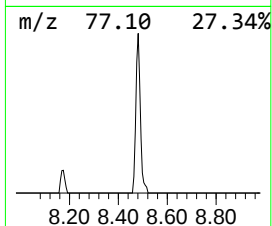
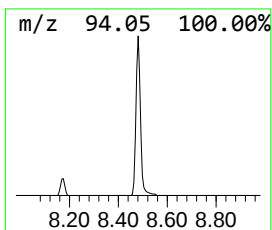
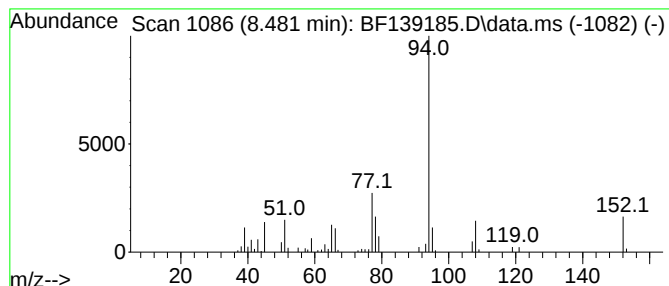
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	2.74 ng	82505	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	59



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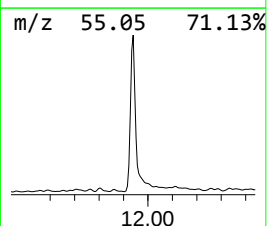
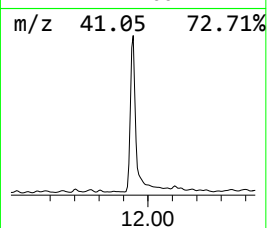
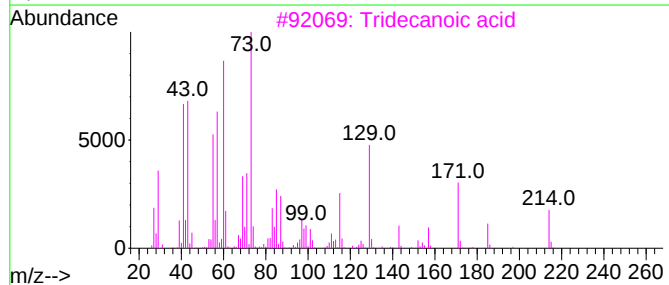
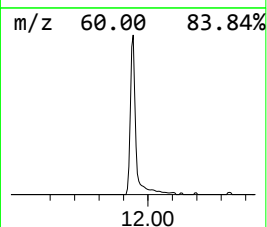
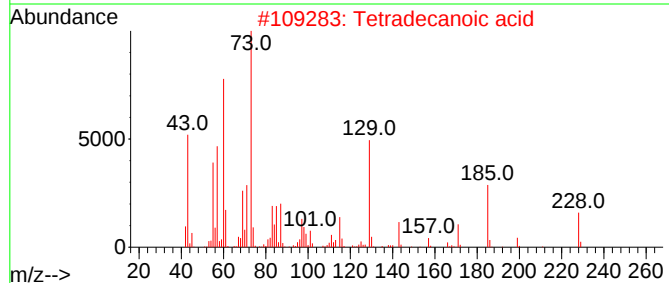
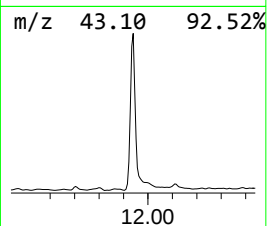
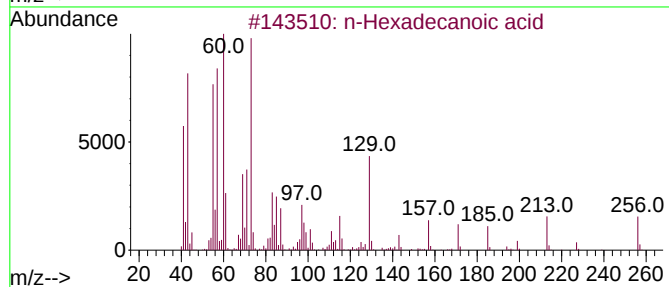
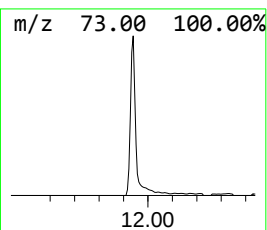
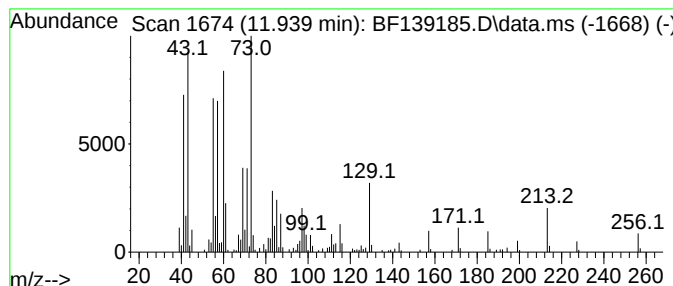
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	9.61 ng	283143	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46



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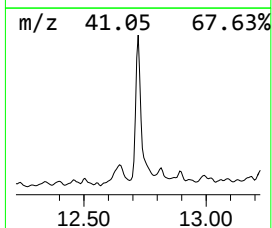
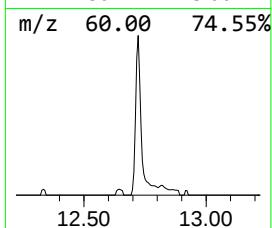
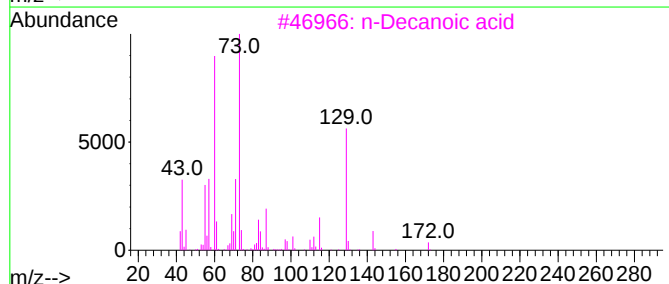
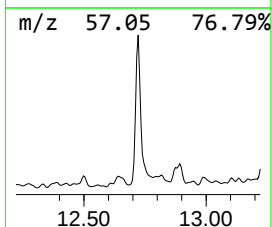
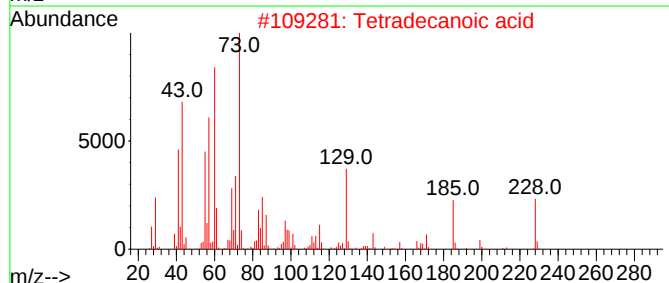
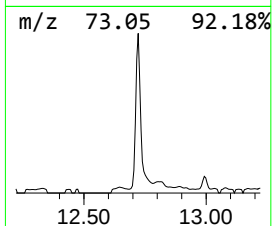
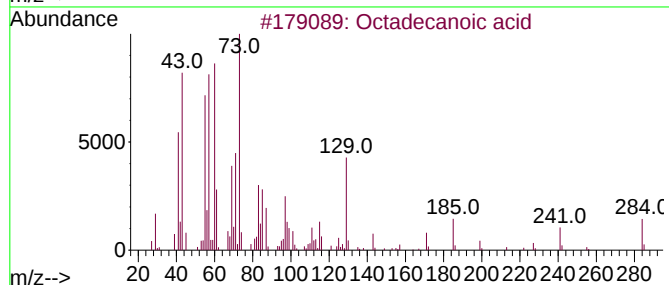
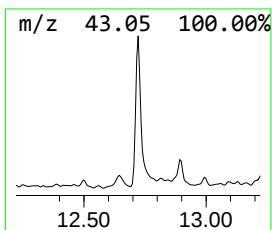
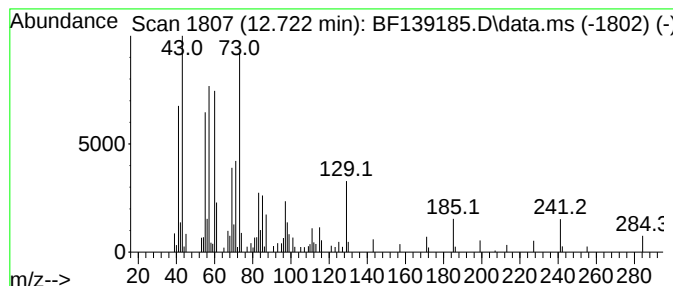
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	4.32 ng	127390	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			n-Decanoic acid	172	C10H20O2	000334-48-5	55
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139185.D
Acq On : 27 Aug 2024 14:17
Operator : RC/JU
Sample : P3717-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

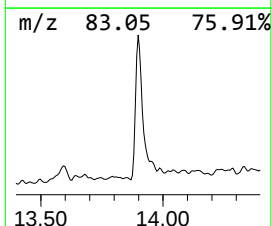
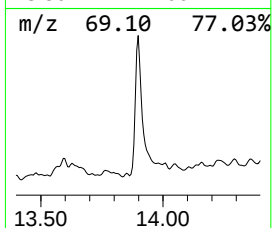
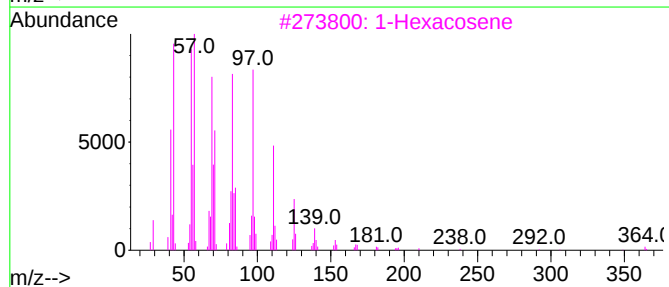
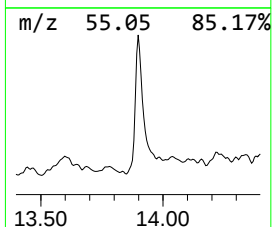
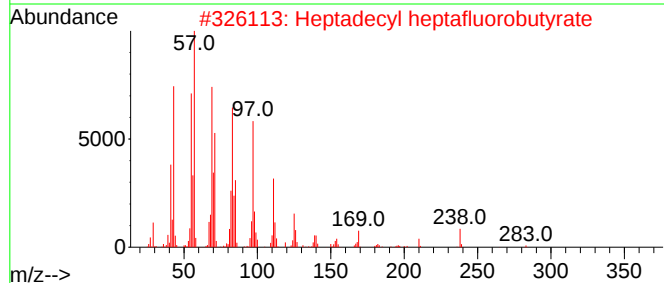
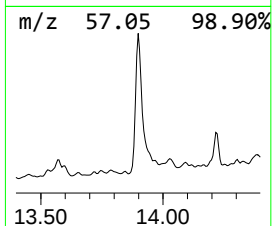
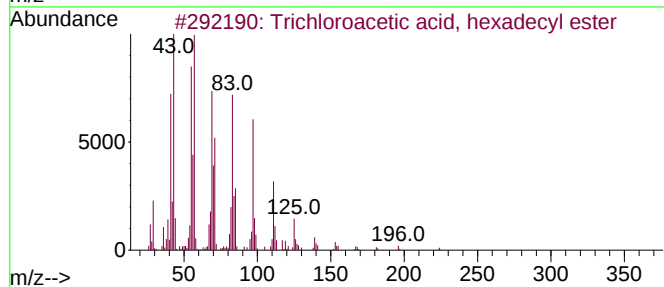
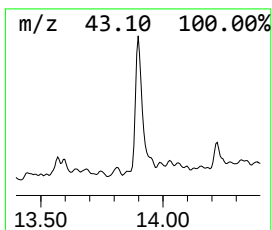
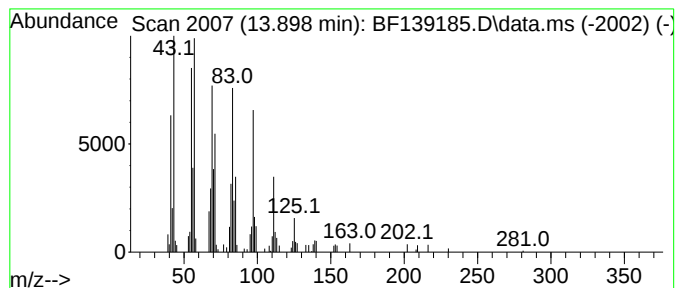
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	4.91 ng	124754	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			1-Tetracosene	336	C24H48	010192-32-2	91
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139185.D
Acq On : 27 Aug 2024 14:17
Operator : RC/JU
Sample : P3717-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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...	2.181	82.3	ng	1993940	1	6.893	484333	20.0
unknown3.381	3.381	2.5	ng	59679	1	6.893	484333	20.0
2-Pentanone, 4-...	5.104	4.5	ng	108261	1	6.893	484333	20.0
1-Phenoxypropan...	8.481	2.7	ng	82505	2	8.175	602292	20.0
n-Hexadecanoic ...	11.939	9.6	ng	283143	4	11.410	589314	20.0
Octadecanoic acid	12.722	4.3	ng	127390	4	11.410	589314	20.0
Trichloroacetic...	13.898	4.9	ng	124754	5	14.045	507664	20.0