

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
 Data File : BF139183.D
 Acq On : 27 Aug 2024 13:16
 Operator : RC/JU
 Sample : P3717-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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: BF139183.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	13	20	rVB	1058409	1602848	98.73%	11.996%
2	3.369	212	217	237	rBV	20036	49085	3.02%	0.367%
3	5.098	502	511	520	rBV	60336	92352	5.69%	0.691%
4	5.504	574	580	585	rBV	1088954	1413524	87.07%	10.579%
5	6.510	745	751	756	rBV	1121465	1454932	89.62%	10.889%
6	6.892	810	816	821	rBV	378960	473013	29.14%	3.540%
7	7.451	905	911	916	rBV	681637	879098	54.15%	6.579%
8	7.704	949	954	958	rBV	27820	32215	1.98%	0.241%
9	8.169	1028	1033	1039	rBV	460449	591300	36.42%	4.425%
10	8.481	1082	1086	1096	rVB	48860	62424	3.85%	0.467%
11	9.245	1211	1216	1221	rBV	1353903	1623491	100.00%	12.150%
12	9.922	1326	1331	1336	rBV	543263	664266	40.92%	4.971%
13	10.016	1341	1347	1353	rBV	25585	38439	2.37%	0.288%
14	10.710	1460	1465	1470	rBV	738043	925538	57.01%	6.927%
15	11.410	1579	1584	1591	rVB	497807	612607	37.73%	4.585%
16	11.939	1668	1674	1690	rBV	180485	280175	17.26%	2.097%
17	12.621	1785	1790	1801	rBV3	18993	49102	3.02%	0.367%
18	12.721	1802	1807	1820	rBV	80928	128453	7.91%	0.961%
19	12.892	1833	1836	1842	rVB3	11160	16636	1.02%	0.125%
20	12.992	1848	1853	1858	rBV	1056229	1333338	82.13%	9.979%
21	13.898	2002	2007	2017	rBV2	44540	96454	5.94%	0.722%
22	14.045	2027	2032	2039	rVB	384938	492515	30.34%	3.686%
23	14.527	2110	2114	2123	rBV3	9486	19189	1.18%	0.144%
24	14.910	2176	2179	2185	rVB	16165	21919	1.35%	0.164%
25	15.180	2221	2225	2229	rBV	12958	18065	1.11%	0.135%
26	15.521	2277	2283	2288	rBV	256918	391011	24.08%	2.926%

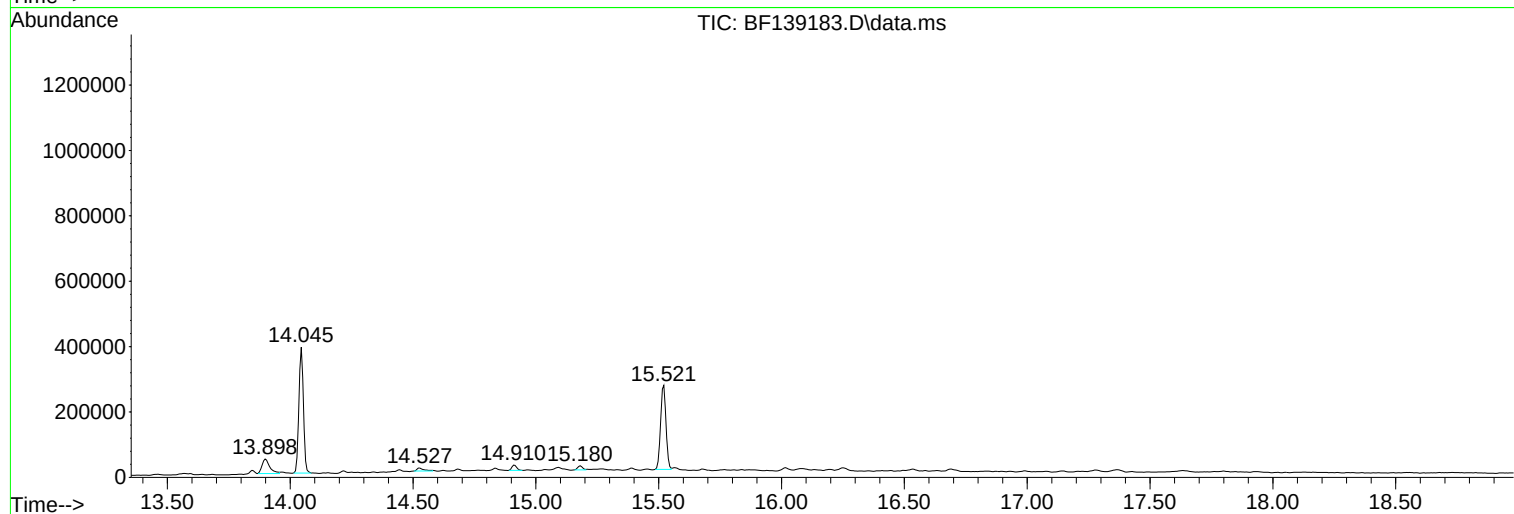
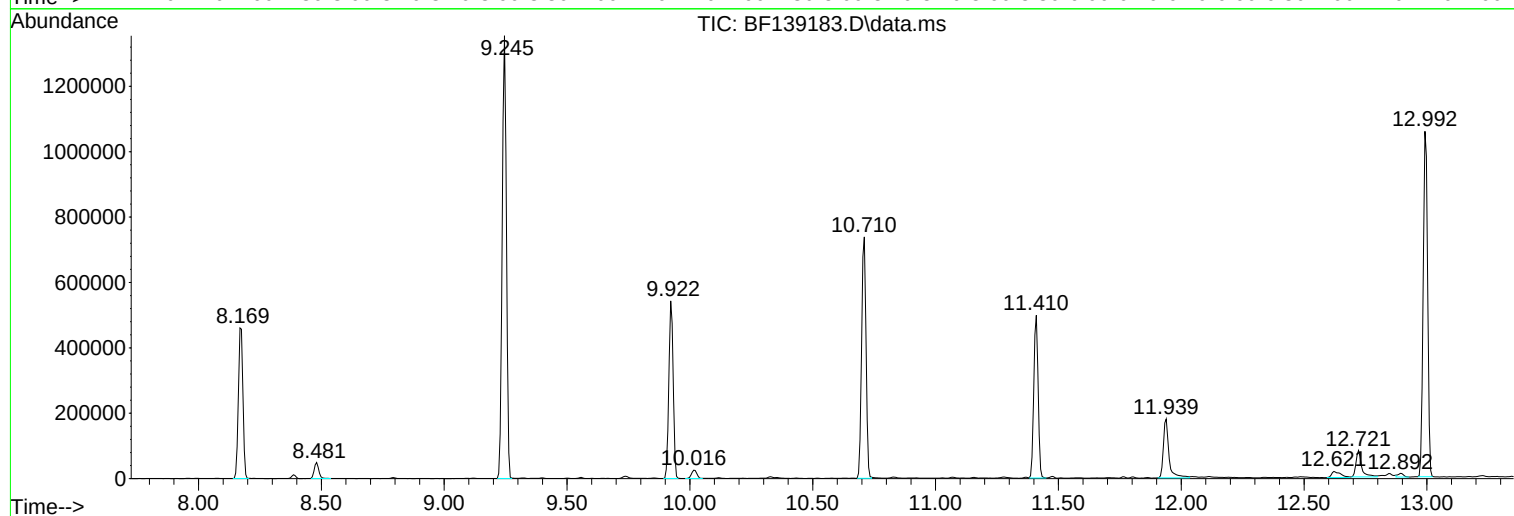
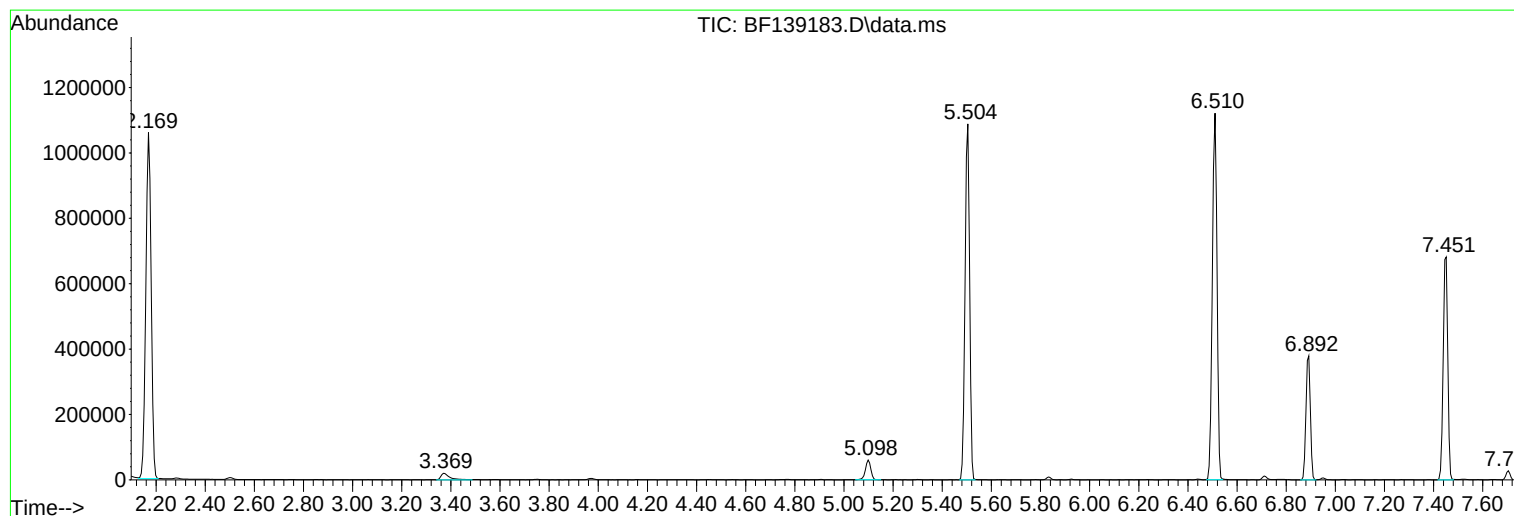
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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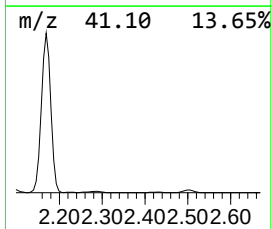
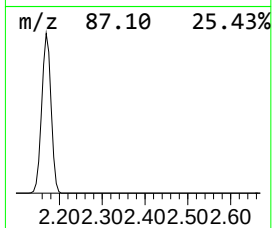
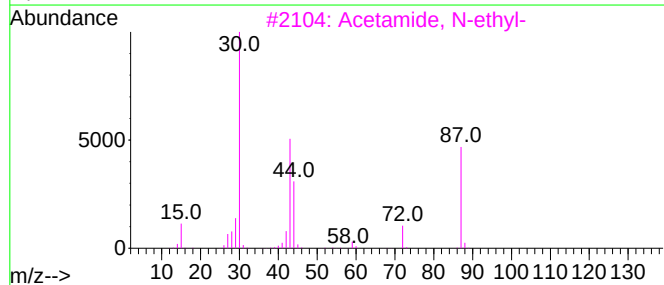
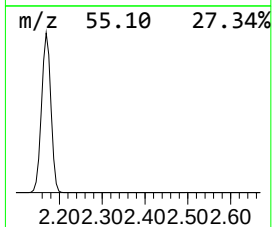
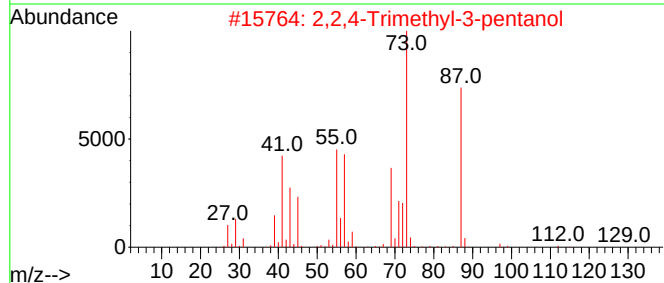
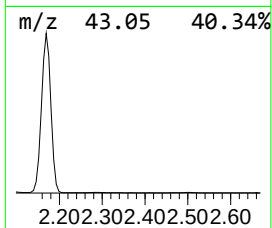
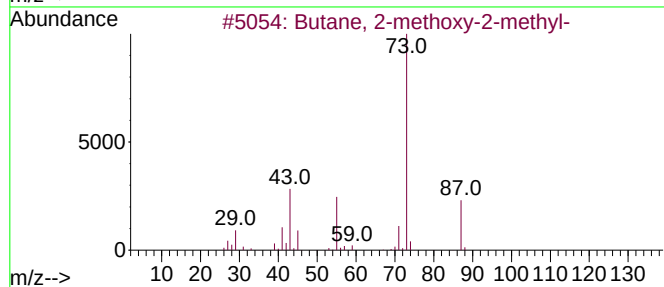
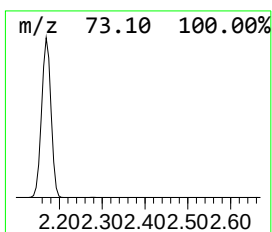
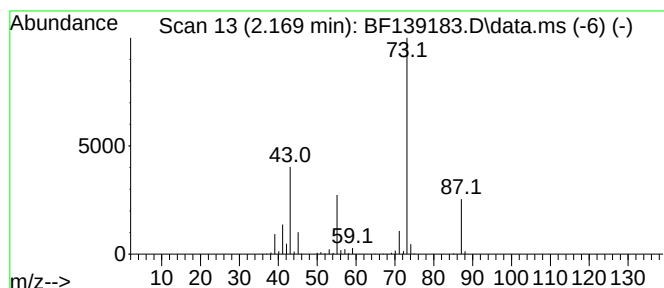
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	67.77 ng	1602850	1,4-Dichlorobenzene-d4	6.892

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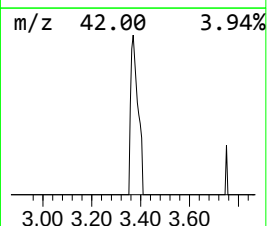
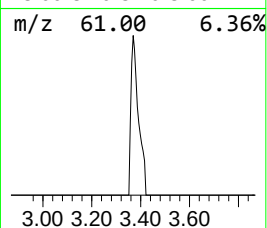
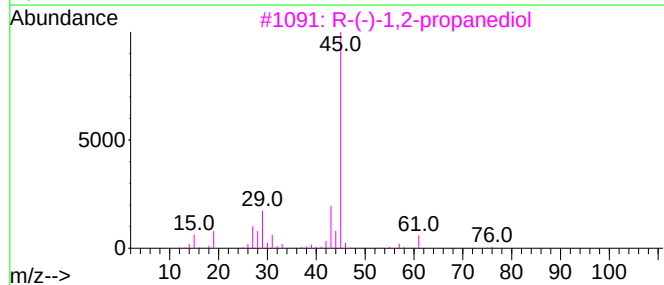
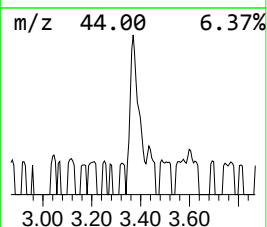
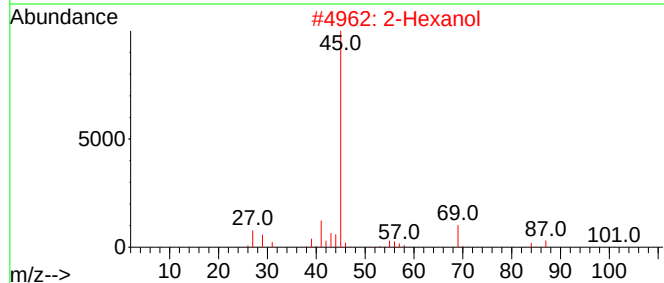
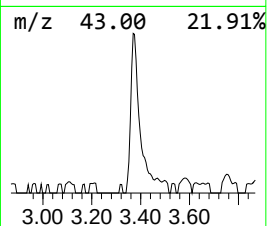
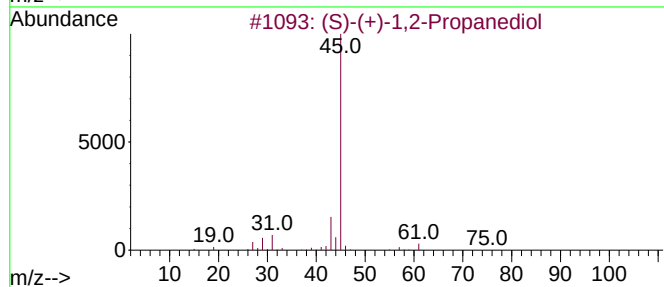
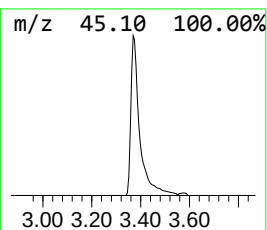
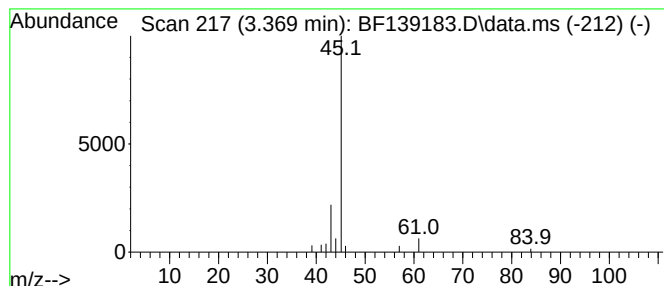
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.369	2.08 ng	49085	1,4-Dichlorobenzene-d4	6.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		2-Hexanol	102	C6H14O	000626-93-7	64
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
4		Propylene Glycol	76	C3H8O2	000057-55-6	9
5		2-Heptanol, (S)-	116	C7H16O	006033-23-4	9



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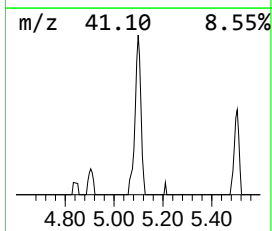
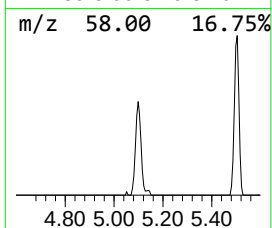
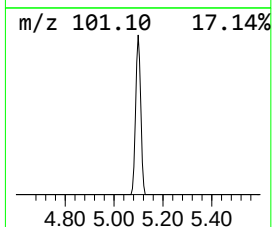
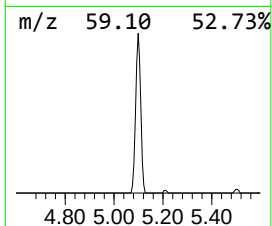
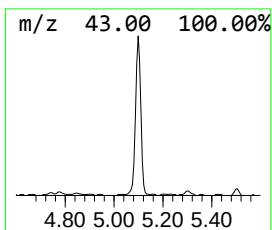
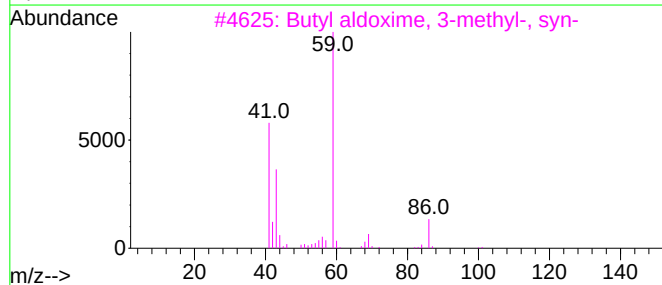
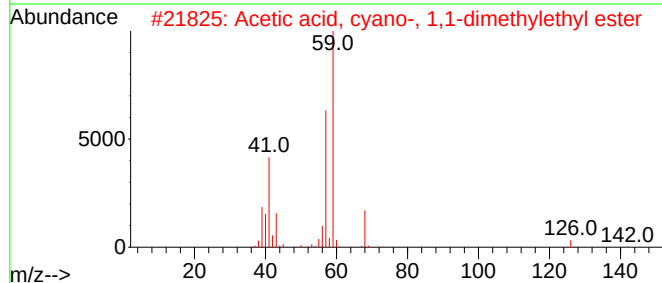
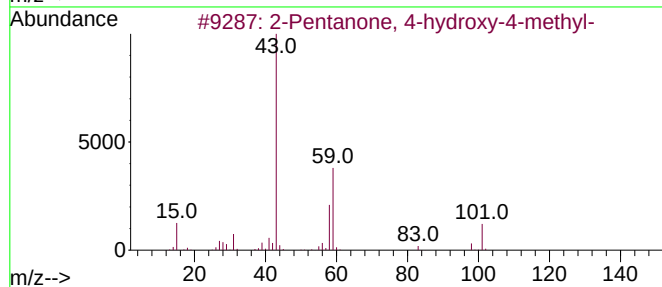
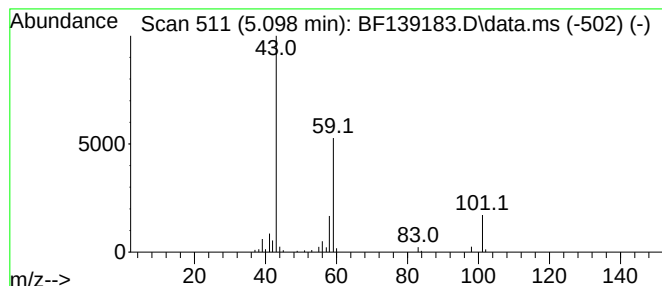
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.90 ng	92352	1,4-Dichlorobenzene-d4	6.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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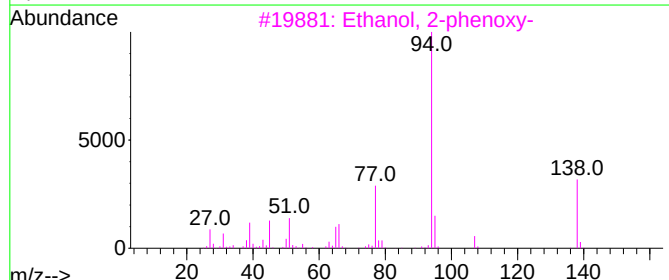
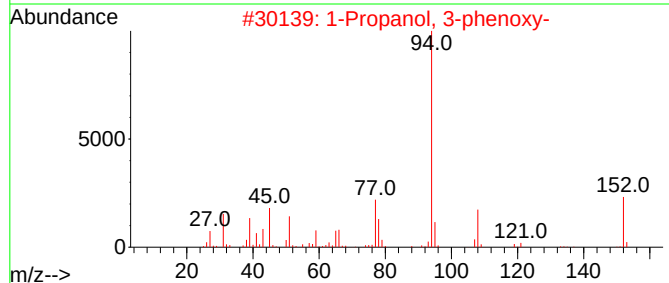
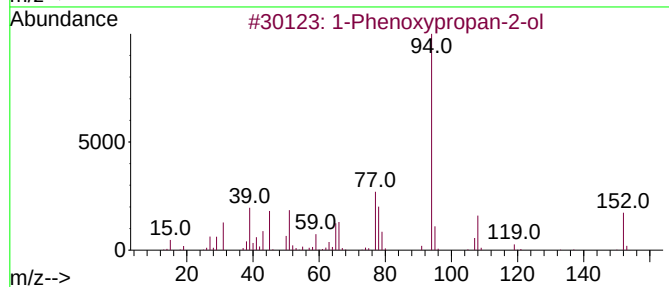
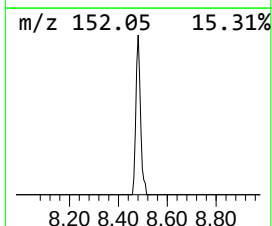
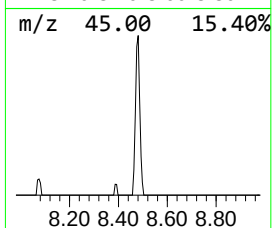
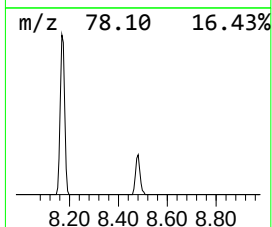
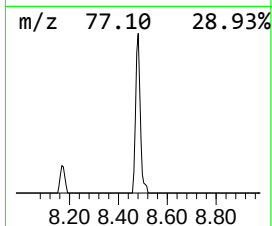
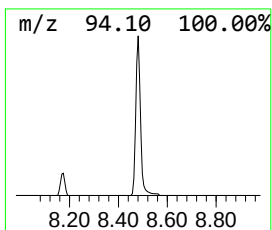
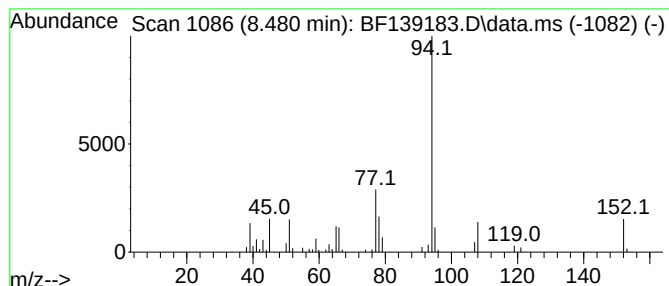
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.480	2.11 ng	62424	Naphthalene-d8	8.175

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	83
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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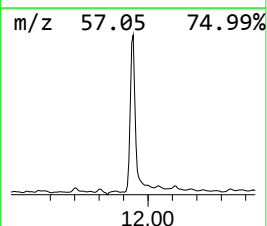
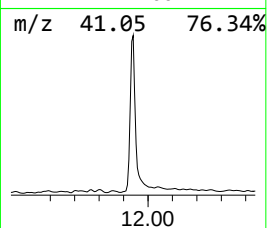
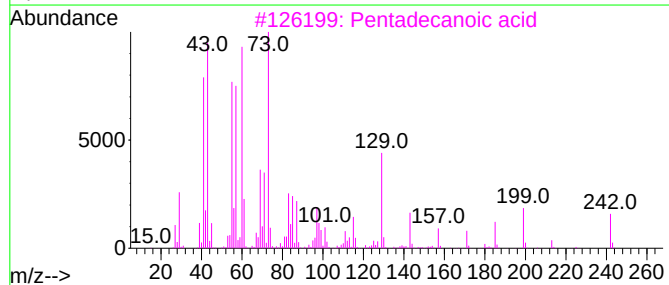
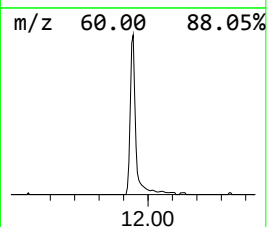
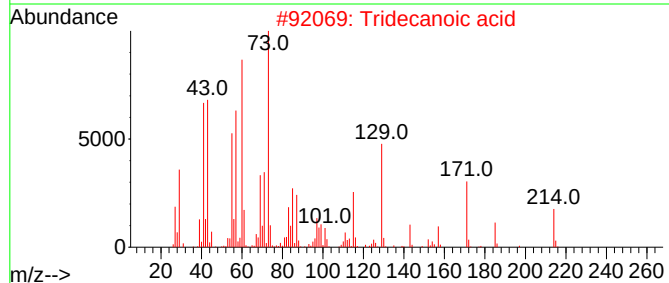
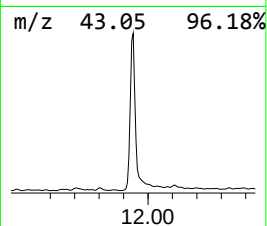
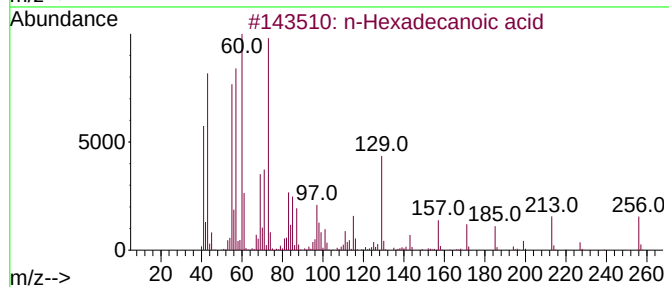
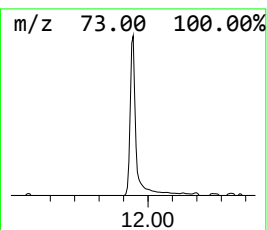
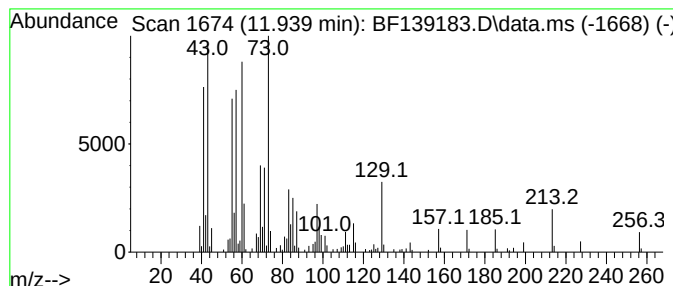
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	9.15 ng	280175	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49
5			Nonanoic acid	158	C9H18O2	000112-05-0	45



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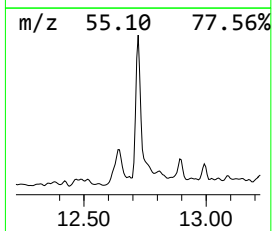
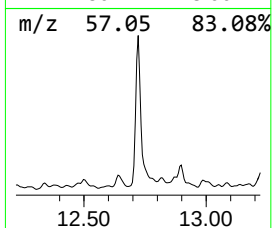
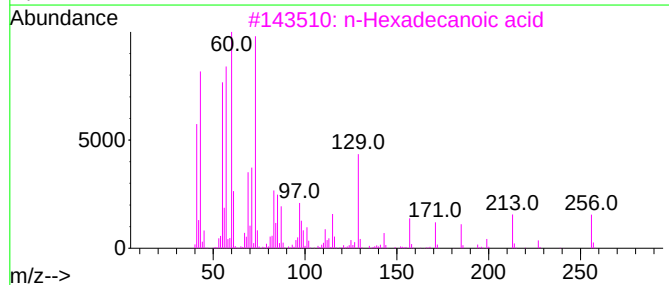
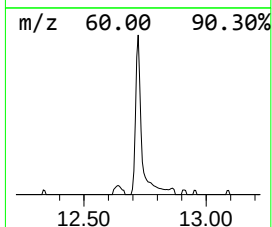
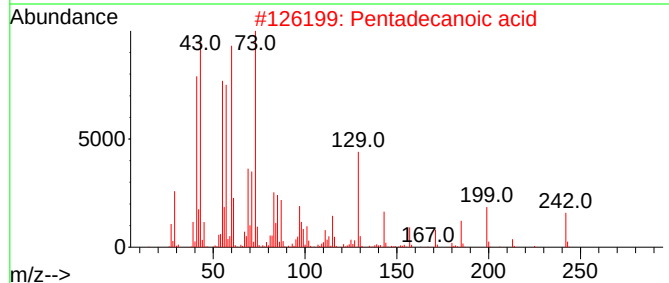
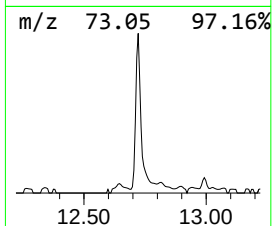
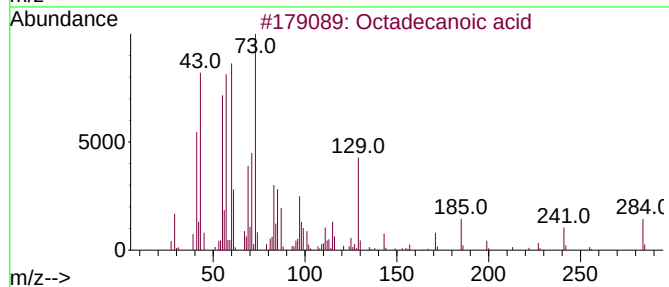
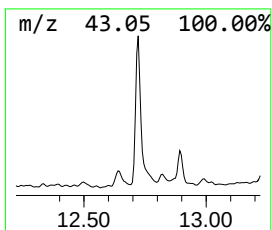
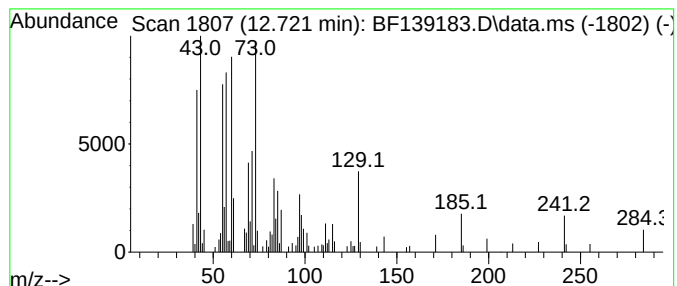
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.721	4.19 ng	128453	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139183.D
Acq On : 27 Aug 2024 13:16
Operator : RC/JU
Sample : P3717-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

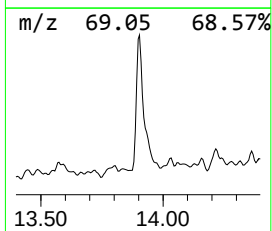
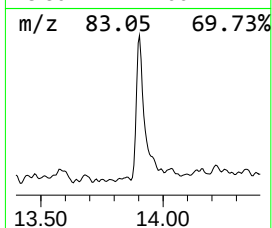
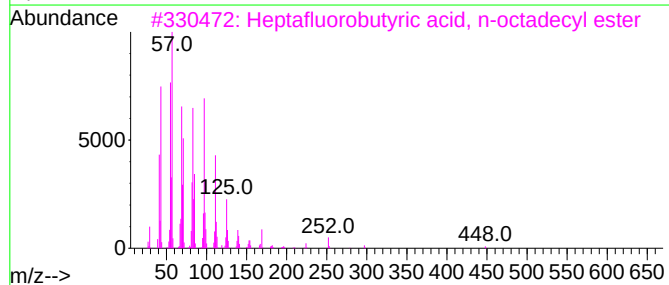
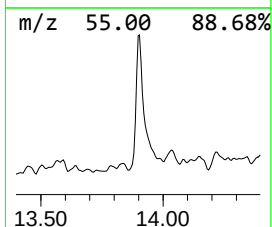
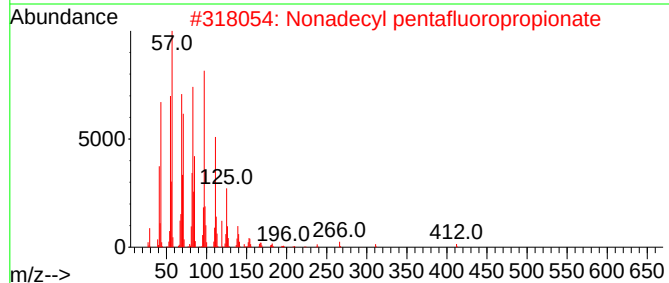
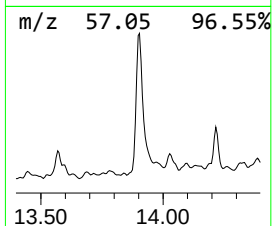
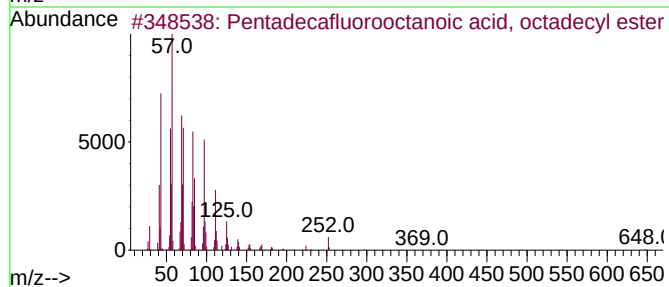
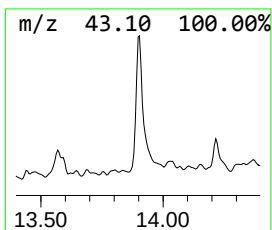
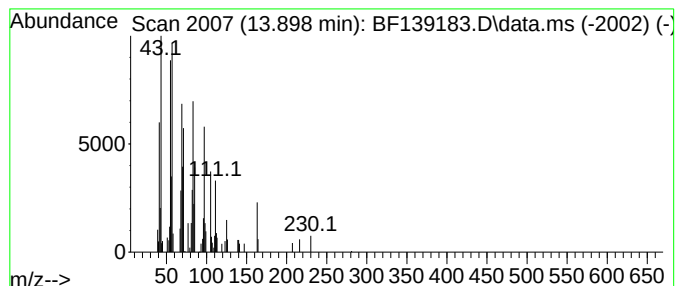
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.92 ng	96454	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
3			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139183.D
Acq On : 27 Aug 2024 13:16
Operator : RC/JU
Sample : P3717-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	67.8	ng	1602850	1	6.892	473013	20.0
(S)-(+)-1,2-Pro...	3.369	2.1	ng	49085	1	6.892	473013	20.0
2-Pentanone, 4-...	5.098	3.9	ng	92352	1	6.892	473013	20.0
1-Phenoxypropan...	8.480	2.1	ng	62424	2	8.175	591300	20.0
n-Hexadecanoic ...	11.939	9.2	ng	280175	4	11.410	612607	20.0
Octadecanoic acid	12.721	4.2	ng	128453	4	11.410	612607	20.0
Pentadecafluoro...	13.898	3.9	ng	96454	5	14.045	492515	20.0