

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030524\
 Data File : BF137504.D
 Acq On : 05 Mar 2024 17:03
 Operator : CG\JU
 Sample : P1672-13
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-13

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137504.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	19	24	36	rVB	40534	69671	1.65%	0.217%
2	3.446	228	231	247	rBV	105990	244670	5.81%	0.763%
3	5.104	508	513	521	rBV	56083	76843	1.82%	0.239%
4	5.499	576	580	603	rBV	3794981	3798636	90.13%	11.839%
5	6.487	744	748	768	rBV	3710794	3991743	94.71%	12.441%
6	6.851	806	810	826	rBV	1052511	1045611	24.81%	3.259%
7	7.410	901	905	917	rBV	2419182	2460633	58.38%	7.669%
8	8.122	1023	1026	1043	rBV	1564966	1396540	33.14%	4.353%
9	8.445	1078	1081	1096	rBV	94999	150448	3.57%	0.469%
10	9.204	1206	1210	1213	rBV	4947137	4214597	100.00%	13.135%
11	9.881	1321	1325	1338	rBV	1946144	1550064	36.78%	4.831%
12	9.986	1338	1343	1353	rBV	1162490	1549829	36.77%	4.830%
13	10.675	1456	1460	1474	rBV	2160222	2068849	49.09%	6.448%
14	10.792	1477	1480	1493	rVB	324734	374126	8.88%	1.166%
15	11.375	1576	1579	1583	rBV	1776561	1483123	35.19%	4.622%
16	11.780	1645	1648	1652	rBV	77252	65244	1.55%	0.203%
17	12.492	1763	1769	1773	rBV2	68448	73285	1.74%	0.228%
18	12.598	1785	1787	1793	rVB	103919	90754	2.15%	0.283%
19	12.827	1820	1826	1829	rBV	101460	122446	2.91%	0.382%
20	12.980	1847	1852	1855	rBV	4162263	3901677	92.58%	12.160%
21	13.216	1888	1892	1896	rBV3	33167	47322	1.12%	0.147%
22	13.469	1930	1935	1947	rBV	473496	632231	15.00%	1.970%
23	13.898	2004	2008	2018	rBV2	167828	238028	5.65%	0.742%
24	14.033	2027	2031	2045	rVB	967152	1092345	25.92%	3.404%
25	14.216	2059	2062	2066	rBV	55870	56404	1.34%	0.176%
26	14.527	2112	2115	2118	rBV	59091	54727	1.30%	0.171%
27	14.851	2167	2170	2180	rVB2	49096	55162	1.31%	0.172%
28	14.927	2180	2183	2188	rBB	48270	50364	1.19%	0.157%
29	15.116	2211	2215	2219	rBV2	30774	51722	1.23%	0.161%
30	15.216	2228	2232	2237	rBV2	46485	60139	1.43%	0.187%
31	15.557	2285	2290	2299	rBV	680055	956166	22.69%	2.980%
32	16.110	2380	2384	2391	rVB2	38026	62457	1.48%	0.195%

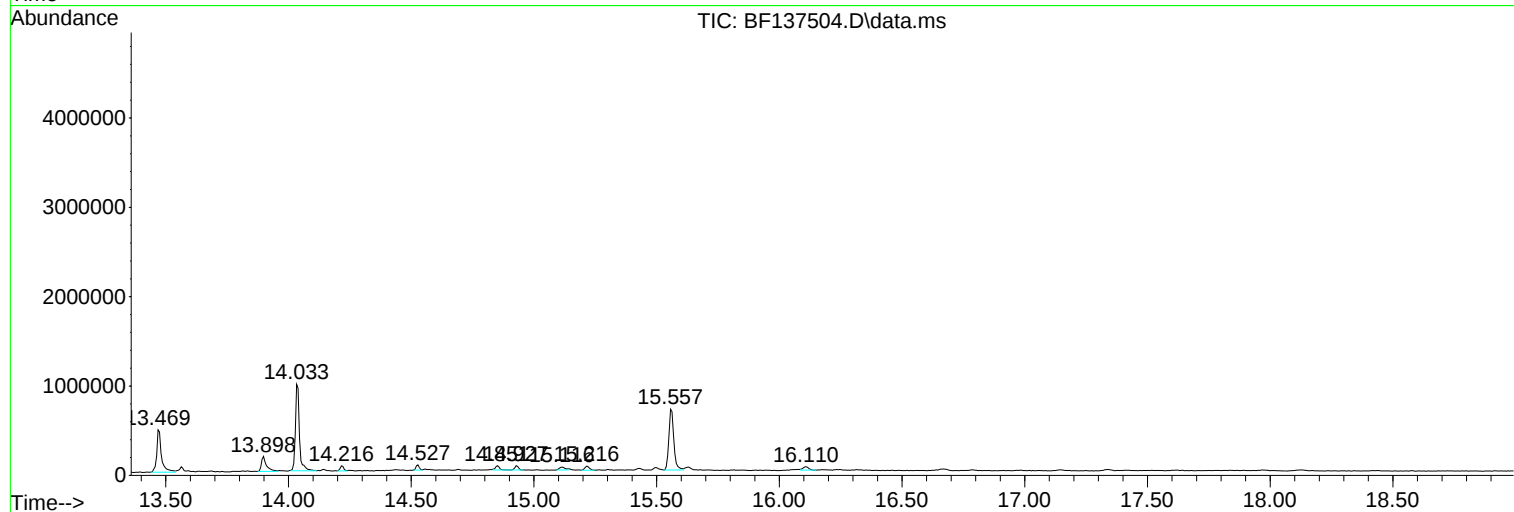
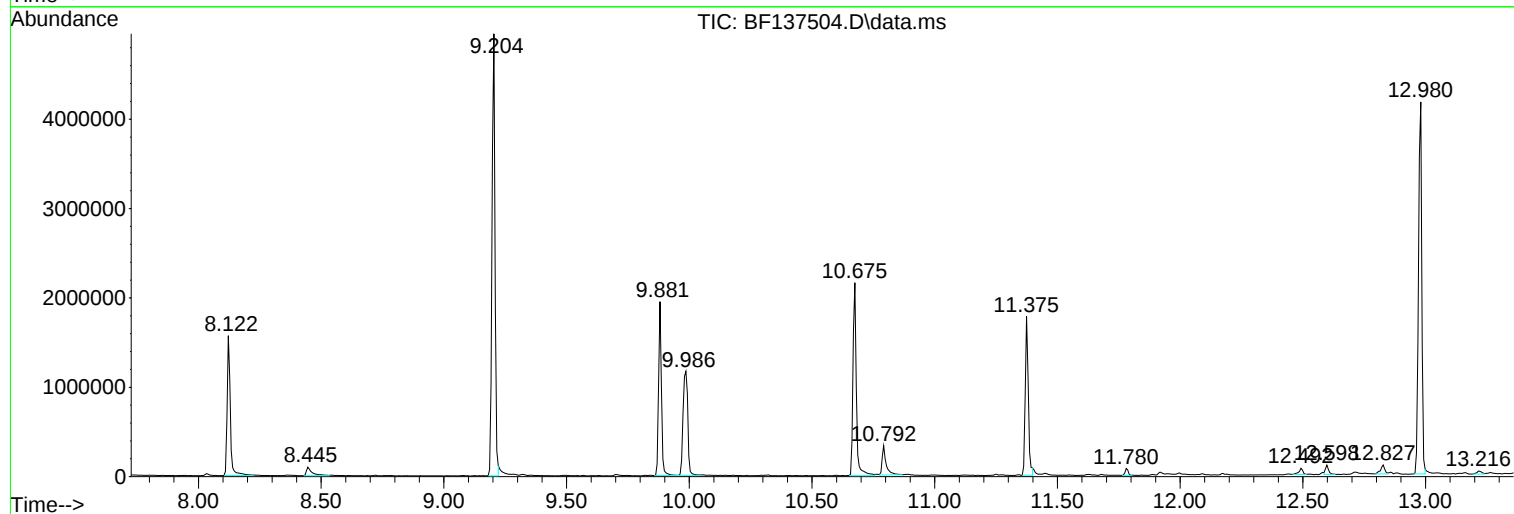
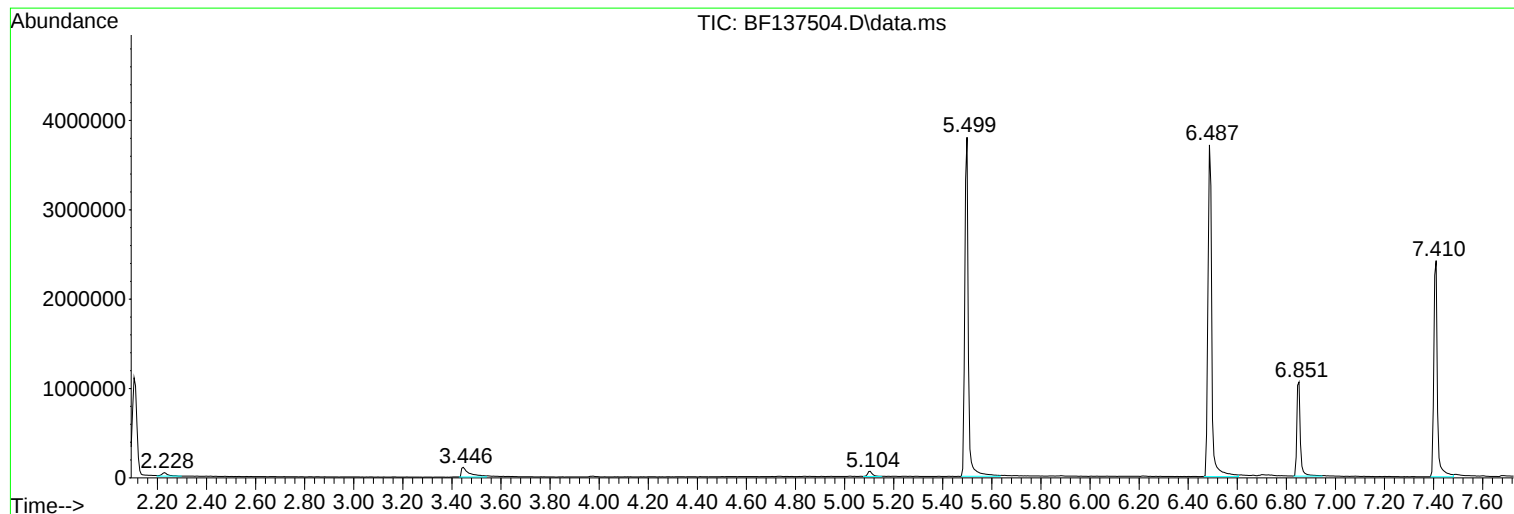
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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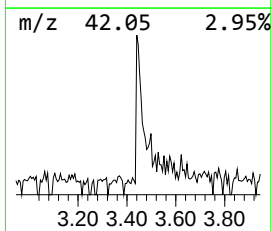
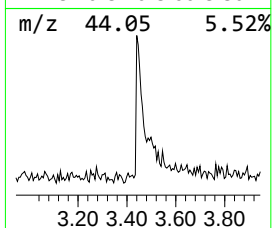
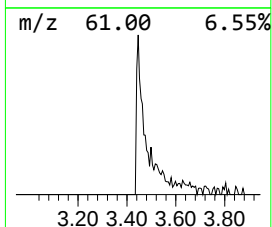
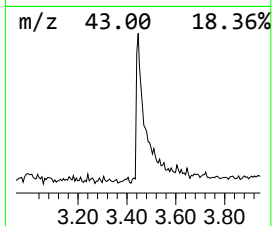
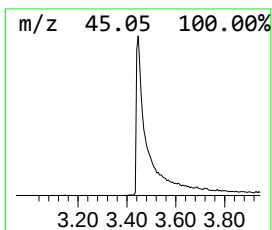
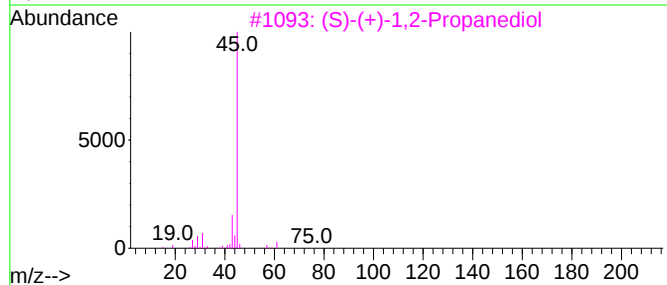
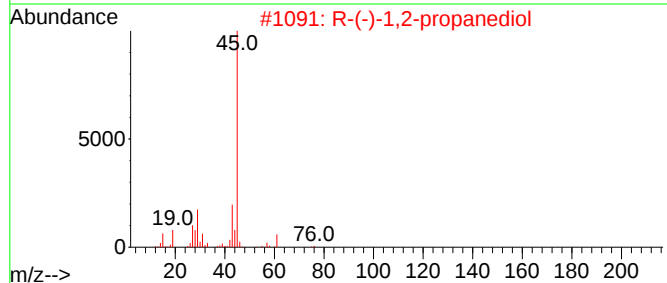
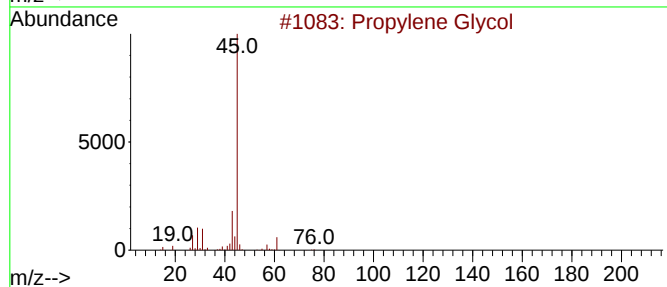
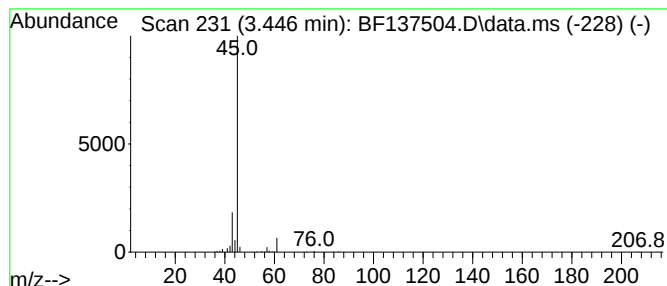
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.446	4.68 ng	244670	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	83
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5			2-Pentanol	88	C5H12O	006032-29-7	9



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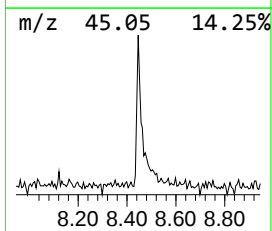
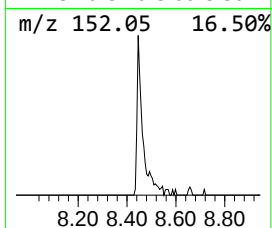
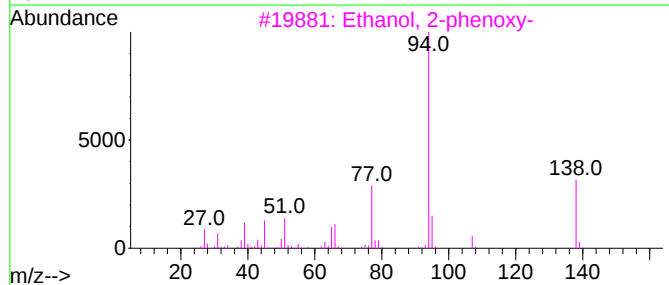
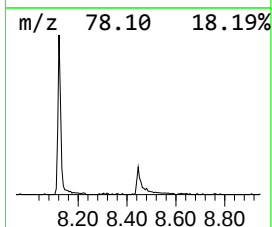
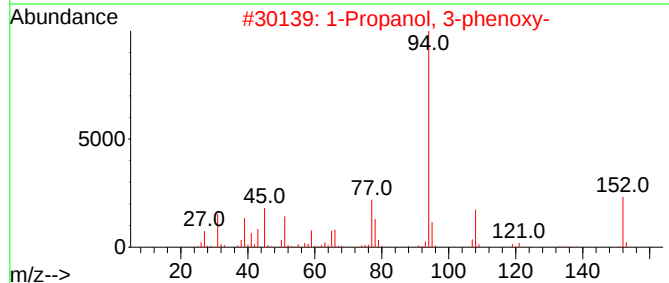
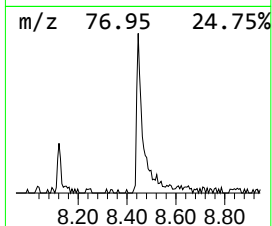
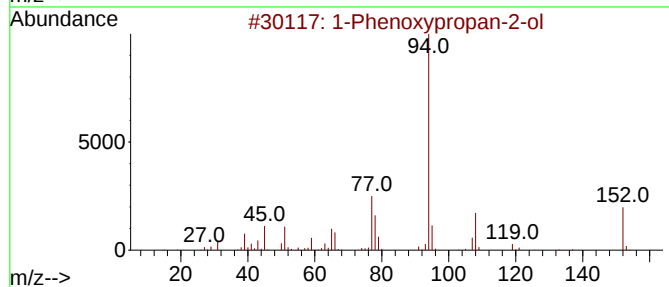
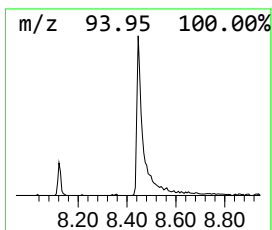
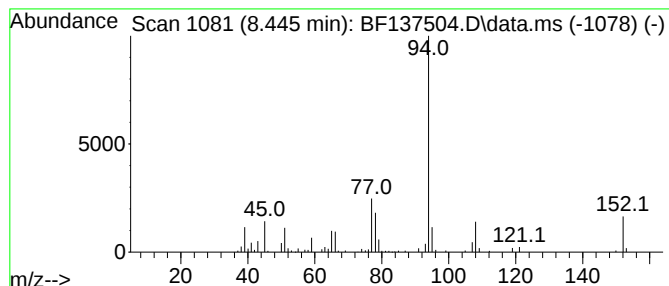
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	2.15 ng	150448	Naphthalene-d8	8.122

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5		3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59



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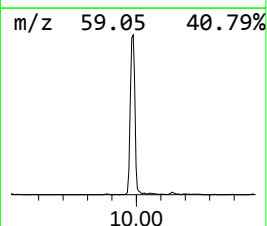
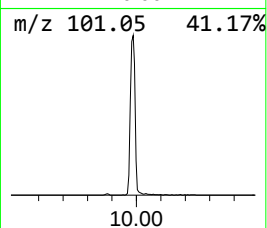
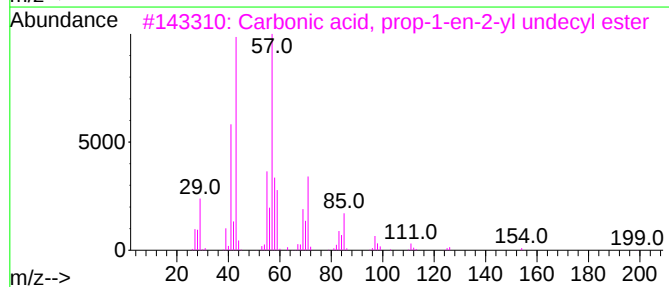
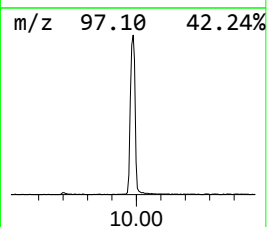
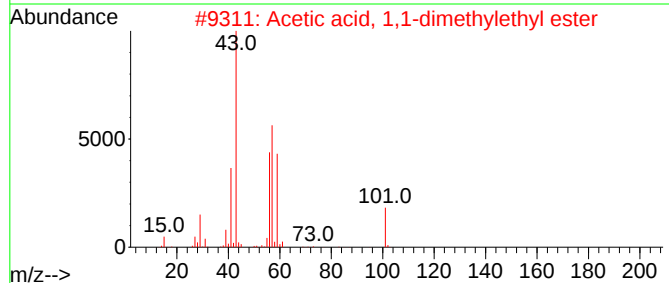
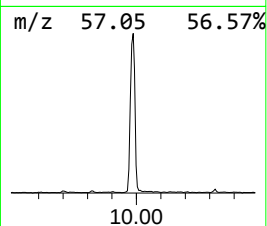
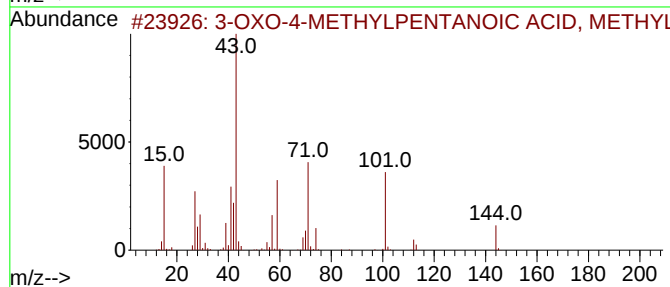
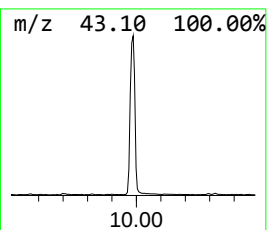
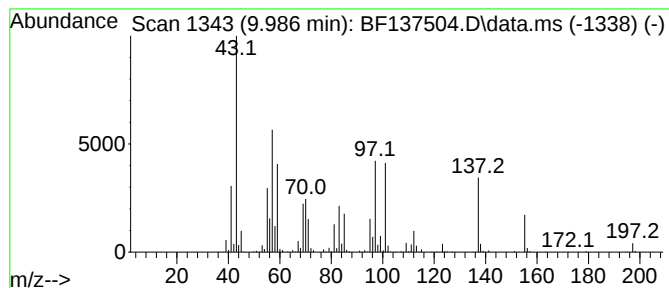
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown9.986 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	20.00 ng	1549830	Acenaphthene-d10	9.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
3			Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	12
4			11-Tricosene	322	C23H46	052078-56-5	12
5			6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	12



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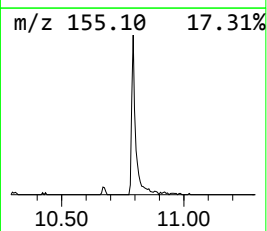
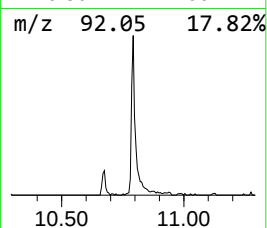
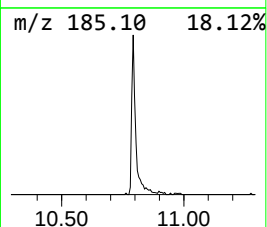
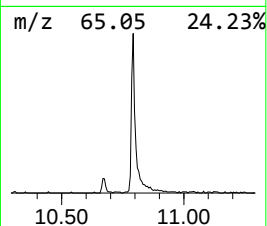
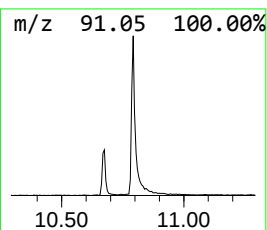
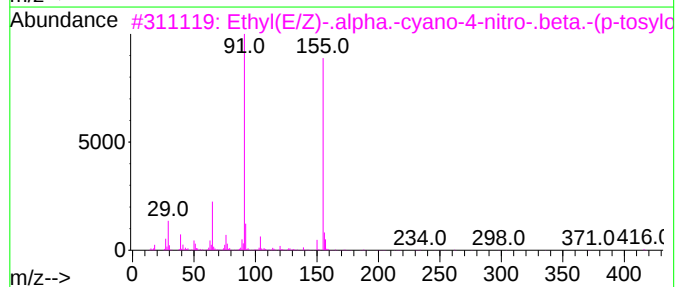
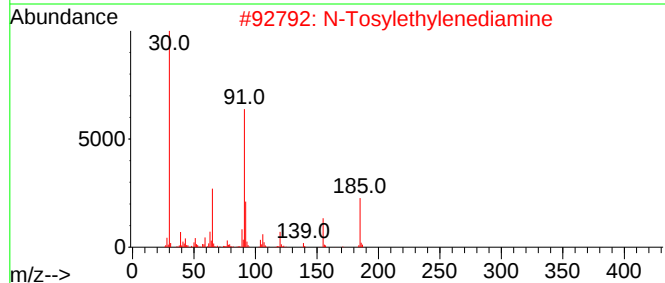
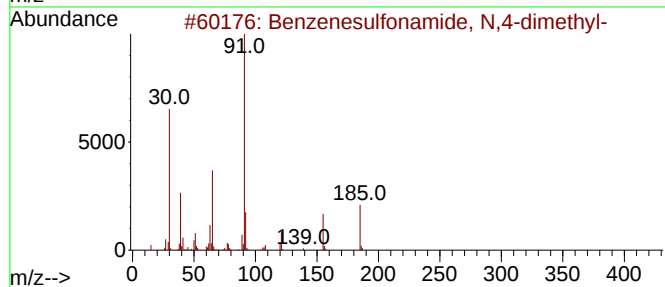
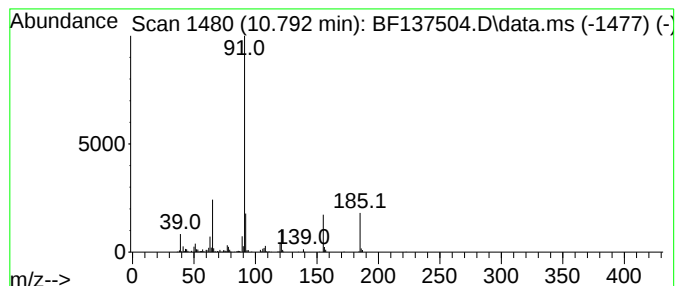
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Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.792	5.05 ng	374126	Phenanthrene-d10	11.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2			N-Tosylethylenediamine	214	C9H14N2O2S	014316-16-6	59
3			Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	53
4			4-Methyl-N-[2-(3-nitro-[1,2,4]tr...	311	C11H13N5O4S	1000301-03-5	50
5			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	50



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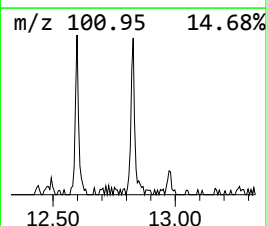
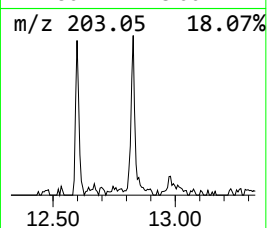
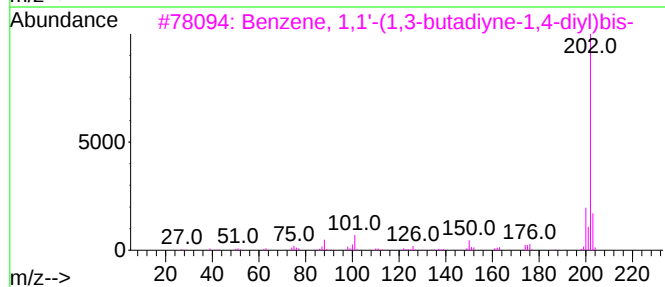
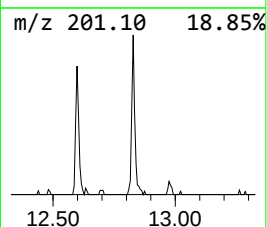
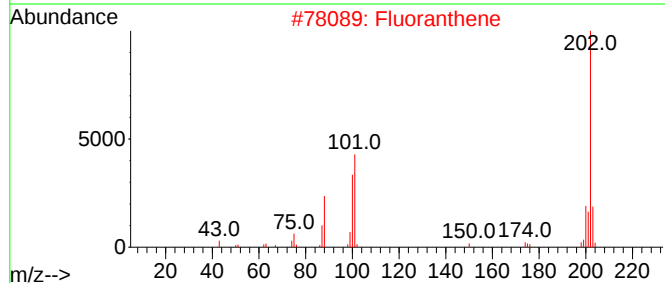
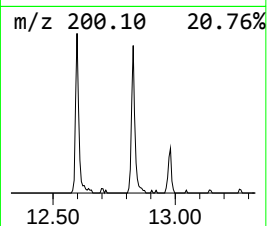
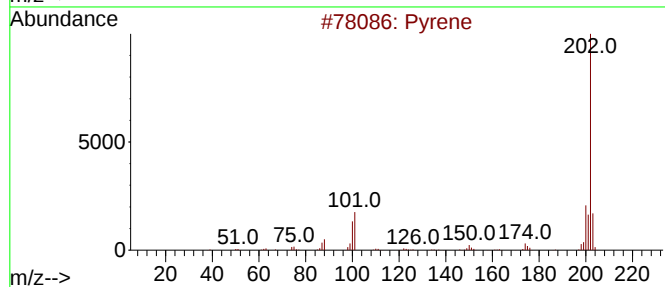
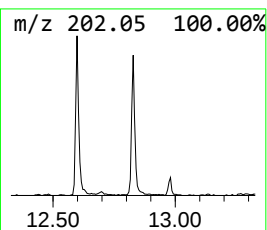
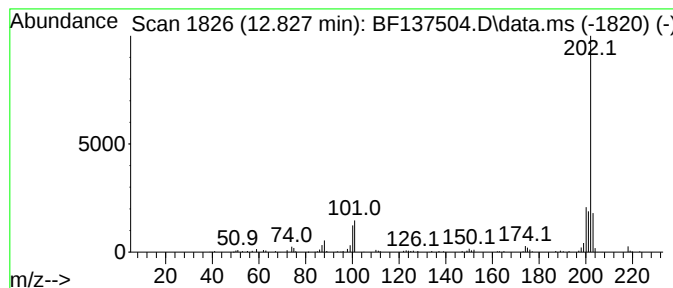
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Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.828	2.24 ng	122446	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	95
2			Fluoranthene	202	C16H10	000206-44-0	93
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	59
4			Benzaldehyde, 2,6-difuloro-3,4-d...	202	C9H8F2O3	152434-99-6	36
5			4,5-Dihydronaphtho(2,1-d)thiazol...	202	C11H10N2S	034176-49-3	36



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Misc :
ALS Vial : 11 Sample Multiplier: 1

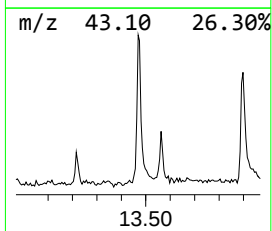
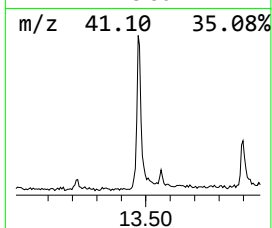
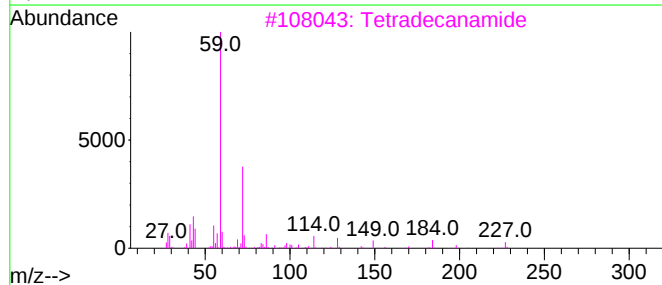
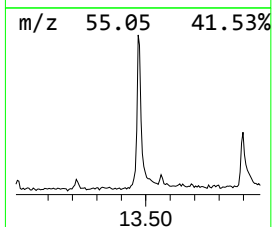
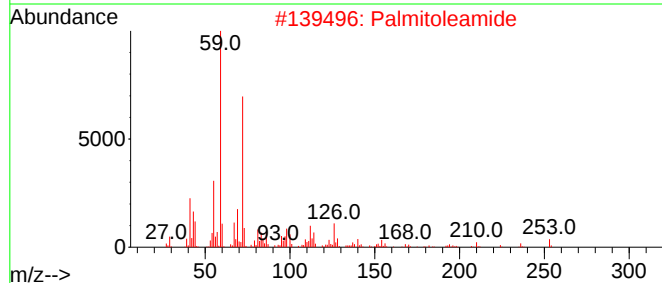
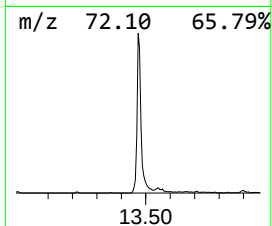
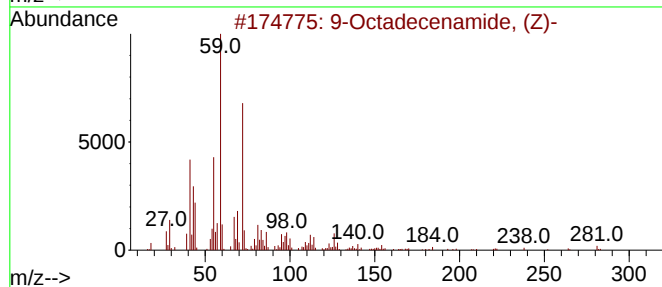
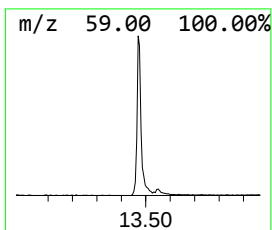
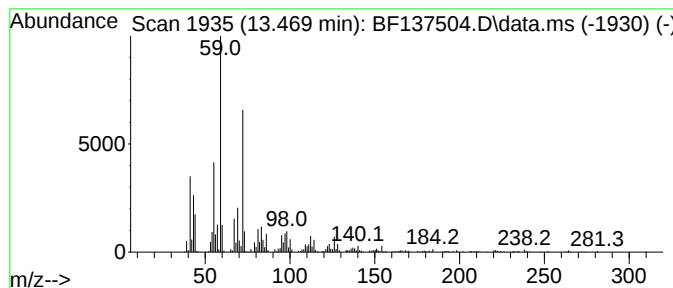
Instrument :
BNA_F
ClientSampleId :
TP-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.469	11.58 ng	632231	Chrysene-d12		14.039	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	98
2	Palmitoleamide		253	C16H31NO	106010-22-4	72
3	Tetradecanamide		227	C14H29NO	000638-58-4	72
4	Dodecanamide		199	C12H25NO	001120-16-7	59
5	Pentanamide, 4-methyl-		115	C6H13NO	001119-29-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030524\
Data File : BF137504.D
Acq On : 05 Mar 2024 17:03
Operator : CG\JU
Sample : P1672-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-13

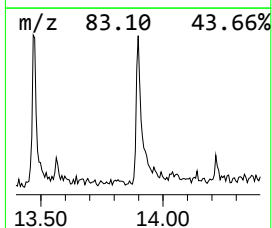
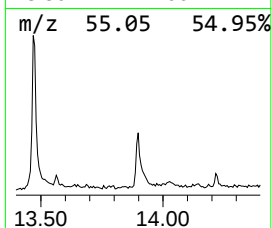
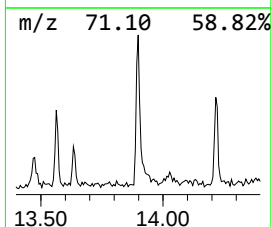
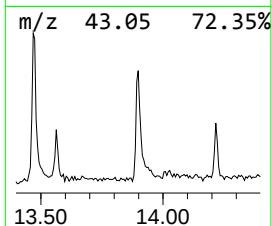
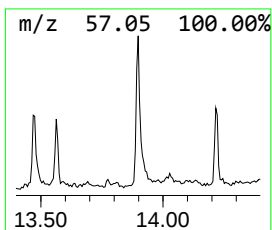
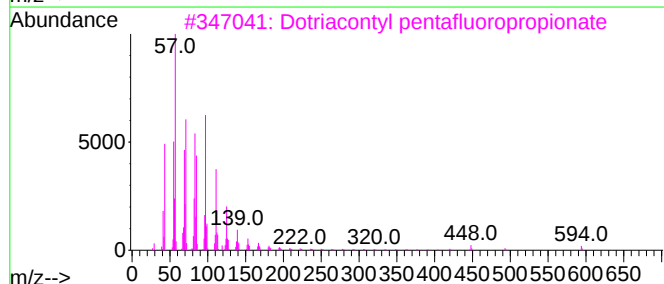
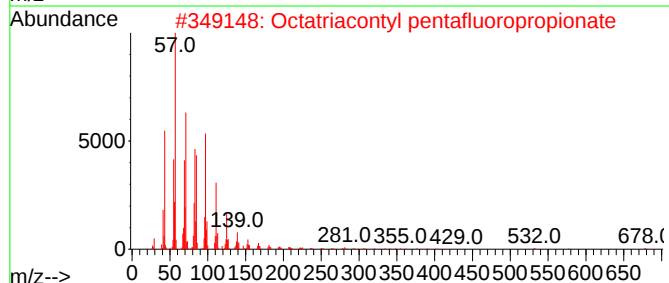
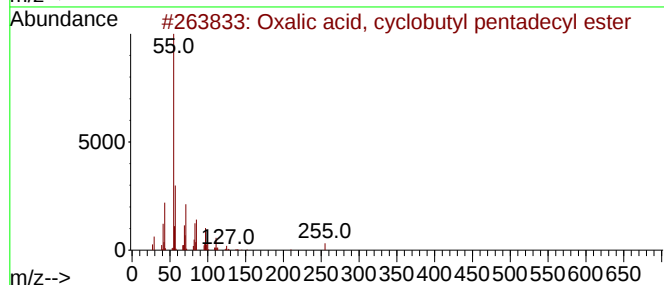
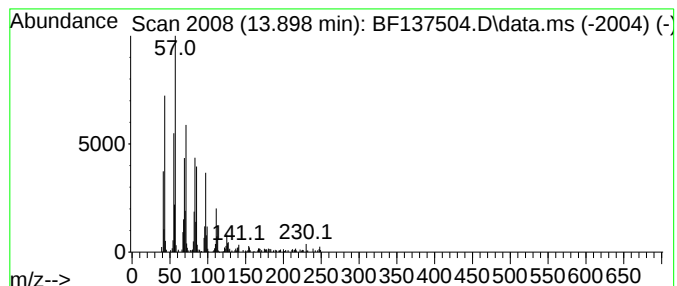
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxalic acid, cyclobutyl pen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	4.36 ng	238028	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	91
2			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91
3			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
4			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
5			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030524\
Data File : BF137504.D
Acq On : 05 Mar 2024 17:03
Operator : CG\JU
Sample : P1672-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
Propylene Glycol	3.446	4.7	ng	244670	1	6.851	1045610	20.0
1-Phenoxypropan...	8.445	2.1	ng	150448	2	8.122	1396540	20.0
unknown9.986	9.986	20.0	ng	1549830	3	9.881	1550060	20.0
Benzenesulfonam...	10.792	5.0	ng	374126	4	11.375	1483120	20.0
Benzene, 1,1'-(...	12.828	2.2	ng	122446	5	14.039	1092350	20.0
9-Octadecenamid...	13.469	11.6	ng	632231	5	14.039	1092350	20.0
Oxalic acid, cy...	13.898	4.4	ng	238028	5	14.039	1092350	20.0