

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102920\
 Data File : BF122165.D
 Acq On : 29 Oct 2020 15:40
 Operator : JU/CG
 Sample : L4547-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TT-033-IDWSO-20201027

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122165.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.210	184	191	209	rBV	174829	517751	14.52%	1.928%
2	5.340	550	553	584	rBV	2661967	3230677	90.63%	12.032%
3	6.369	724	728	755	rBV	2814646	3483108	97.71%	12.972%
4	6.710	783	786	796	rVB	729082	637881	17.89%	2.376%
5	7.287	879	884	900	rBV	2029877	2138458	59.99%	7.964%
6	7.998	1001	1005	1013	rBV	806670	832187	23.35%	3.099%
7	8.434	1076	1079	1089	rVB	52206	82511	2.31%	0.307%
8	9.069	1182	1187	1190	rBV	3141964	3062017	85.90%	11.404%
9	9.269	1217	1221	1230	rBV	202063	336952	9.45%	1.255%
10	9.469	1249	1255	1262	rBV	504635	457911	12.85%	1.705%
11	9.745	1298	1302	1311	rVB	1046388	1010452	28.35%	3.763%
12	10.392	1405	1412	1418	rBV	38151	61821	1.73%	0.230%
13	10.545	1433	1438	1447	rBV	2261372	2450575	68.75%	9.126%
14	10.657	1452	1457	1464	rVV	71419	92169	2.59%	0.343%
15	11.092	1526	1531	1533	rBV5	27678	36870	1.03%	0.137%
16	11.122	1533	1536	1543	rVB	60350	74314	2.08%	0.277%
17	11.233	1551	1555	1565	rBV	1146363	1041212	29.21%	3.878%
18	11.763	1639	1645	1653	rBV3	89662	130723	3.67%	0.487%
19	12.251	1721	1728	1729	rBV2	22608	39502	1.11%	0.147%
20	12.822	1819	1825	1828	rBV	3674240	3564674	100.00%	13.276%
21	13.039	1857	1862	1869	rBV	42242	54083	1.52%	0.201%
22	13.257	1895	1899	1901	rBV2	42907	61736	1.73%	0.230%
23	13.292	1901	1905	1911	rVB	119210	169177	4.75%	0.630%
24	13.380	1916	1920	1923	rBV2	52394	51334	1.44%	0.191%
25	13.710	1970	1976	1992	rBV2	326391	688264	19.31%	2.563%
26	13.880	2001	2005	2014	rVB	985749	977173	27.41%	3.639%
27	14.027	2025	2030	2032	rBV	54299	52239	1.47%	0.195%
28	14.174	2049	2055	2065	rBV4	33990	116564	3.27%	0.434%
29	14.327	2078	2081	2084	rBV	57521	62027	1.74%	0.231%
30	14.369	2084	2088	2095	rVB6	20273	43450	1.22%	0.162%
31	14.627	2128	2132	2136	rVB	54739	55070	1.54%	0.205%
32	14.692	2138	2143	2150	rVV	58555	73241	2.05%	0.273%
33	14.945	2181	2186	2190	rBV	51311	59513	1.67%	0.222%
34	15.316	2241	2249	2261	rBV	651597	919190	25.79%	3.423%
35	15.698	2310	2314	2321	rVB	33378	46853	1.31%	0.174%
36	15.780	2322	2328	2332	rBV6	37902	91105	2.56%	0.339%

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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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.163	2389	2393	2399	rbV4	25726	48504	1.36%	0.181%
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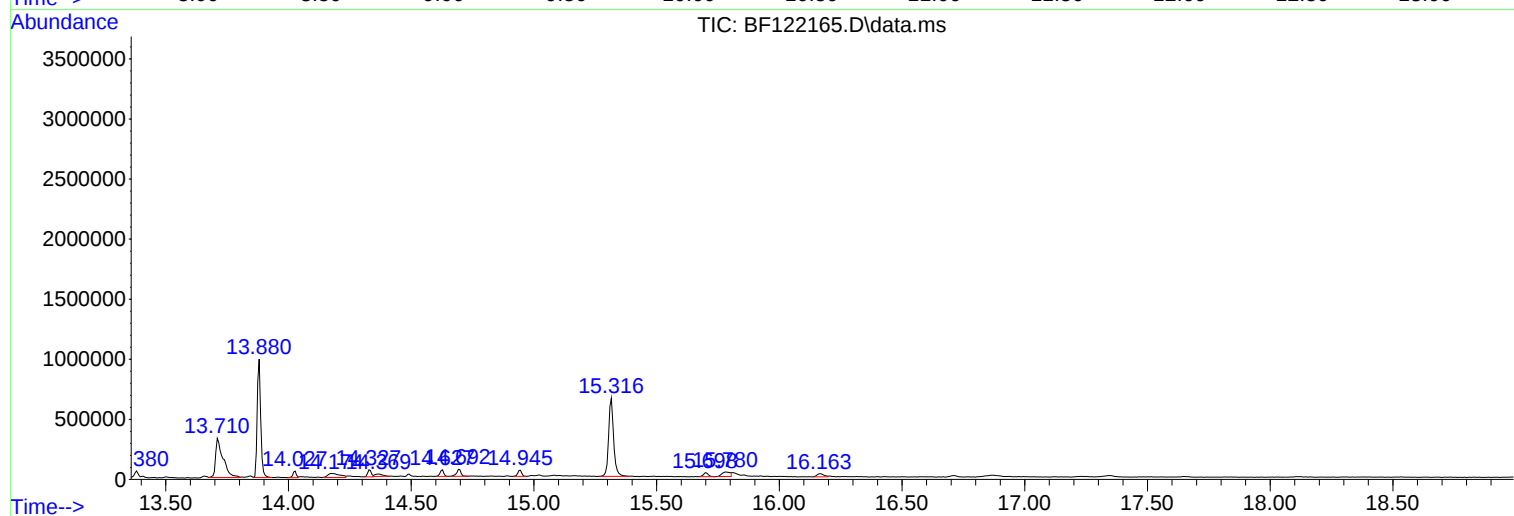
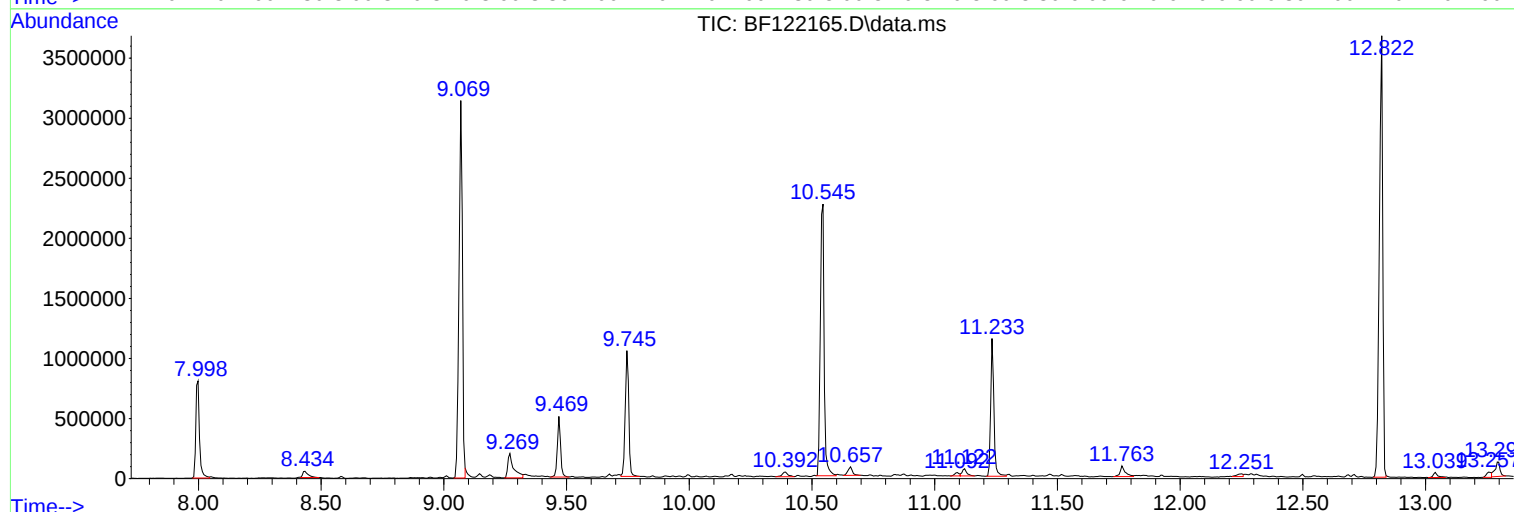
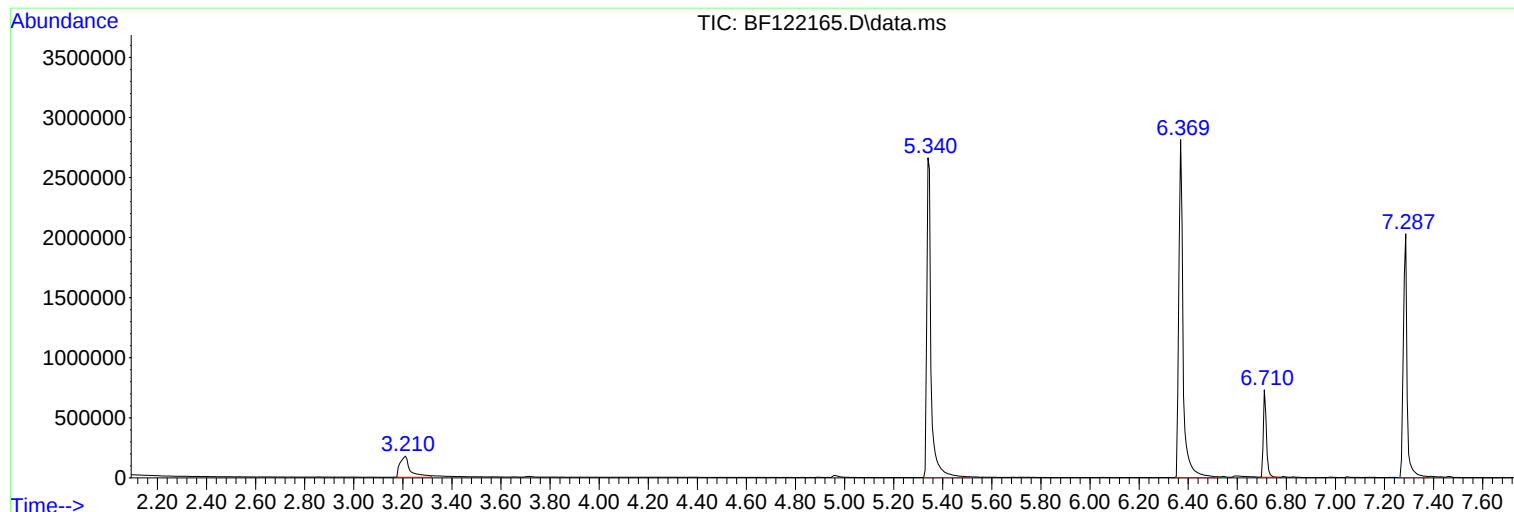
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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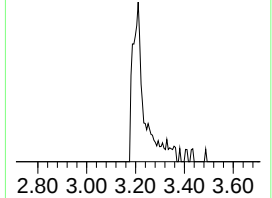
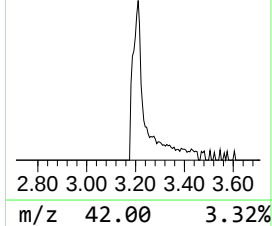
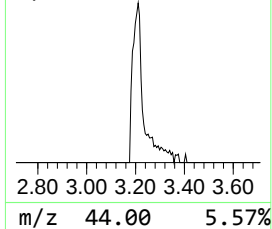
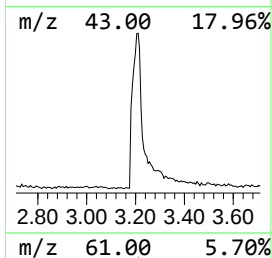
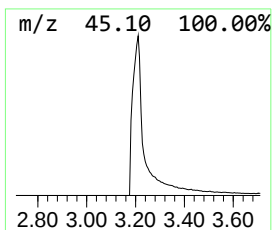
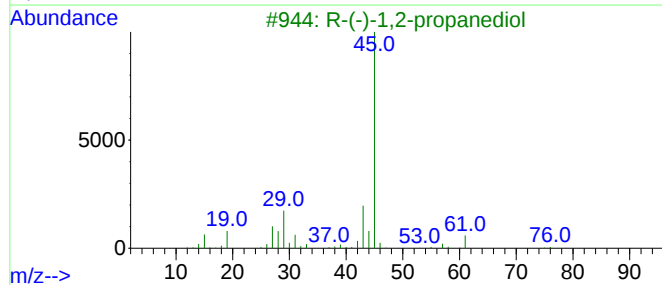
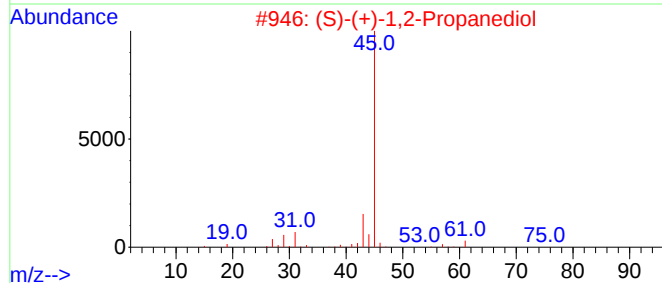
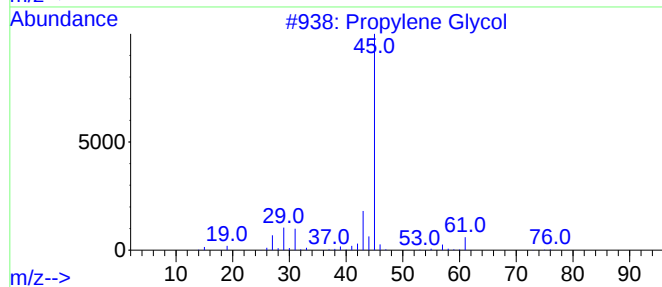
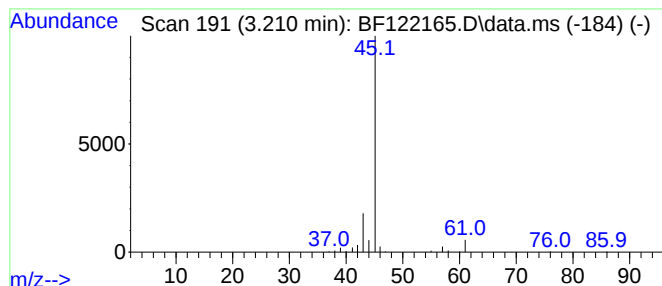
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.210	16.23 ng	517751	1,4-Dichlorobenzene-d4	6.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4			2-Pentanol	88	C5H12O	006032-29-7	9
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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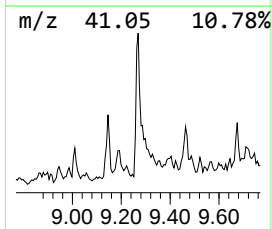
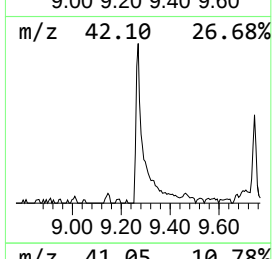
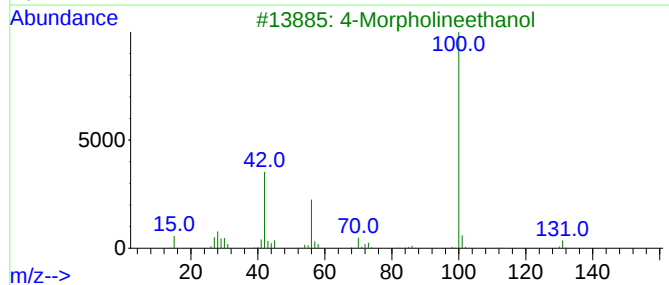
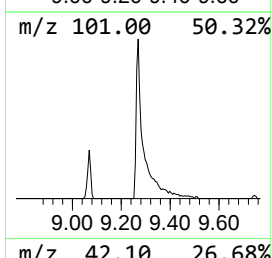
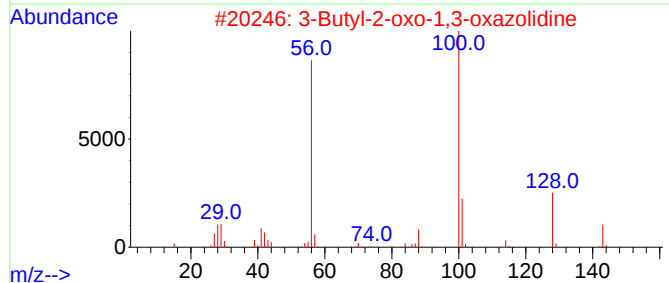
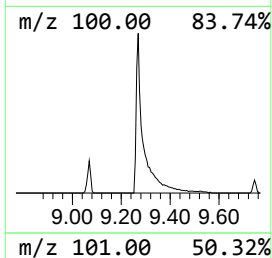
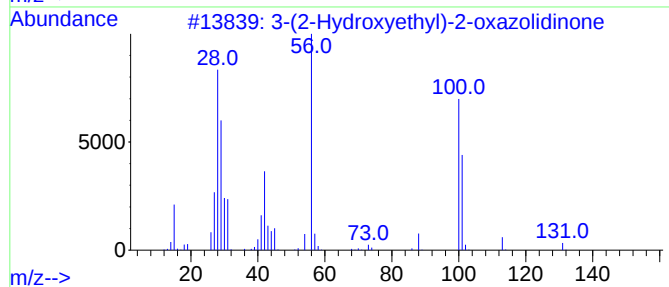
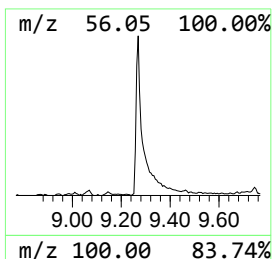
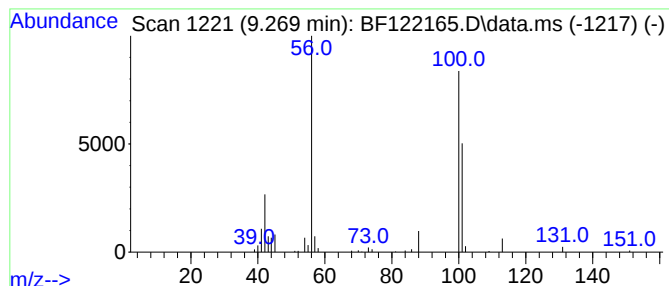
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.269	6.67 ng	336952	Acenaphthene-d10	9.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	91
2			3-Butyl-2-oxo-1,3-oxazolidine	143	C7H13NO2	023288-01-9	38
3			4-Morpholineethanol	131	C6H13NO2	000622-40-2	38
4			1-Butanol	74	C4H10O	000071-36-3	27
5			Aminothiazole	100	C3H4N2S	000096-50-4	10



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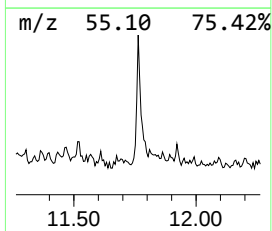
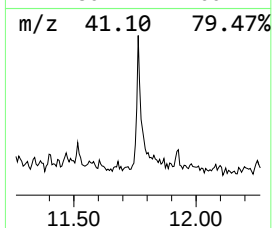
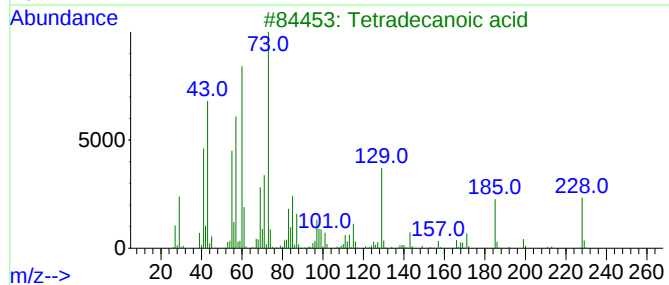
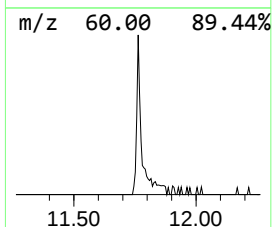
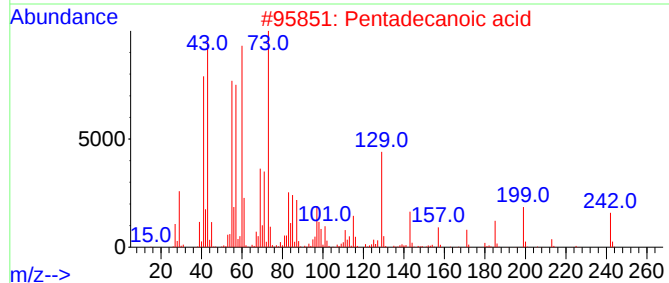
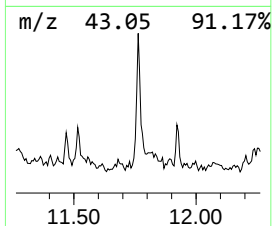
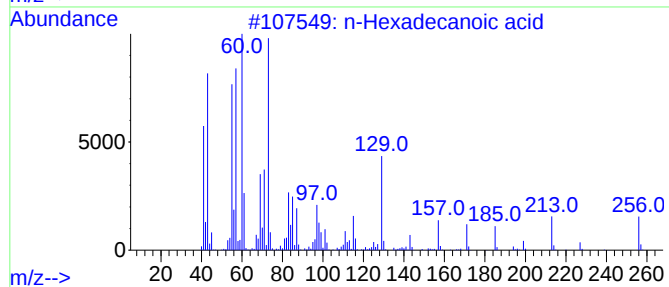
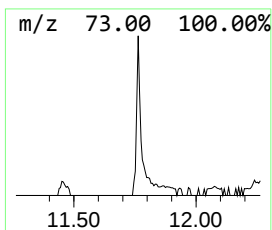
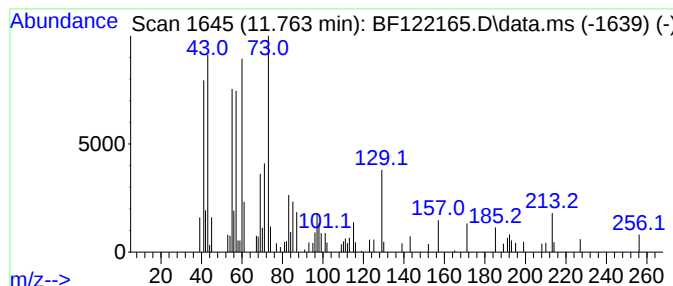
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.763	2.51 ng	130723	Phenanthrene-d10	11.233

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	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	72



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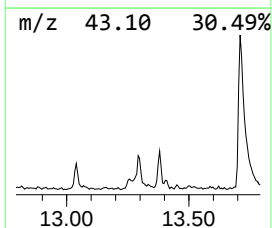
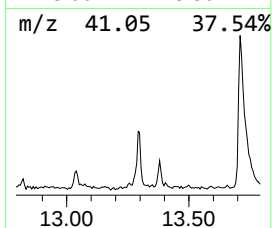
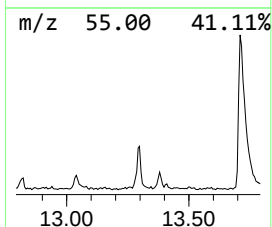
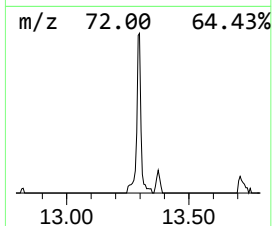
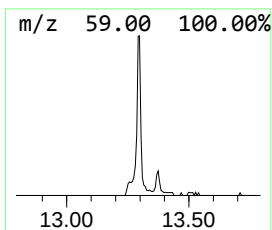
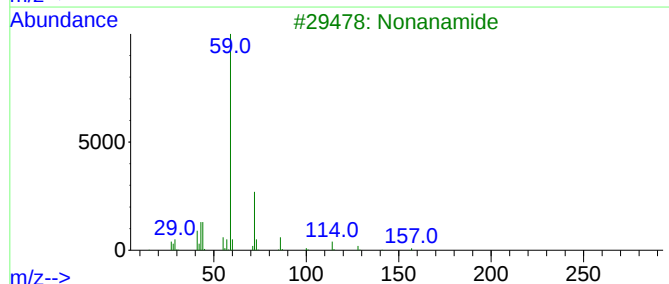
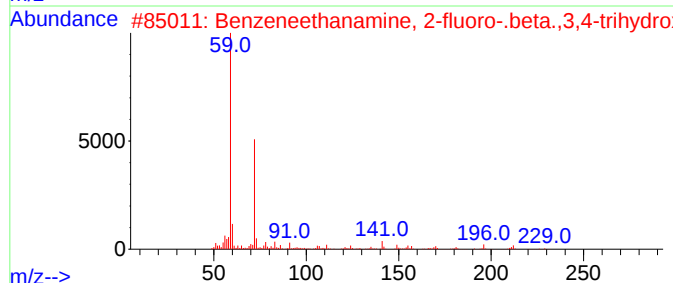
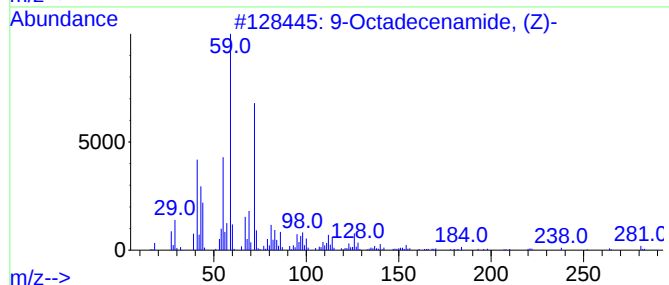
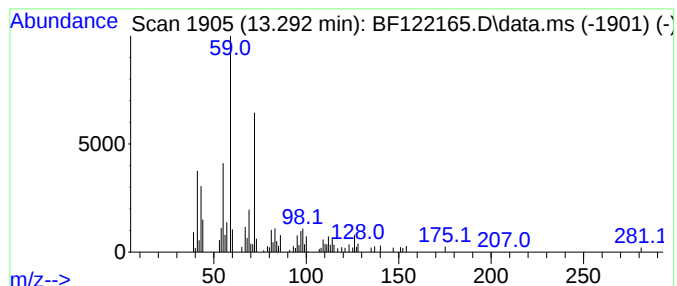
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	3.46 ng	169177	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
3			Nonanamide	157	C9H19NO	001120-07-6	53
4			Hexadecanamide	255	C16H33NO	000629-54-9	53
5			Dodecanamide	199	C12H25NO	001120-16-7	53



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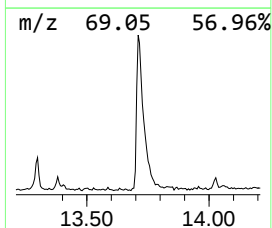
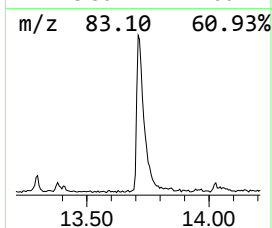
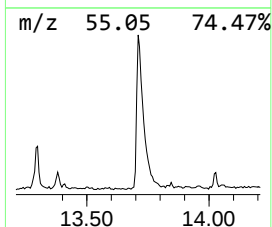
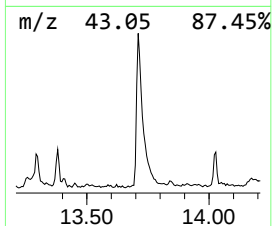
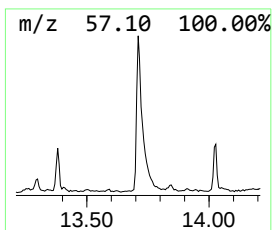
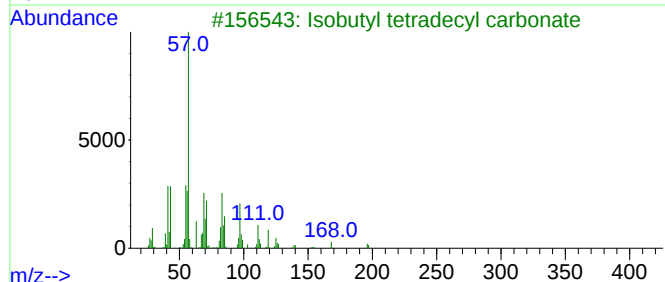
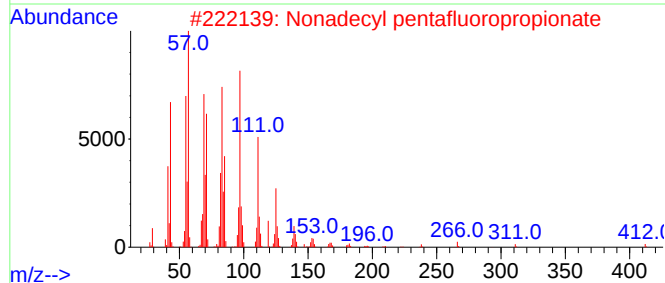
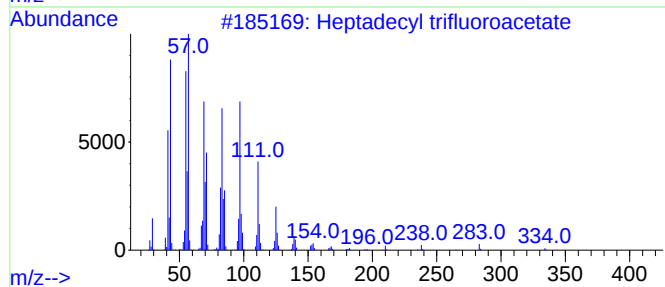
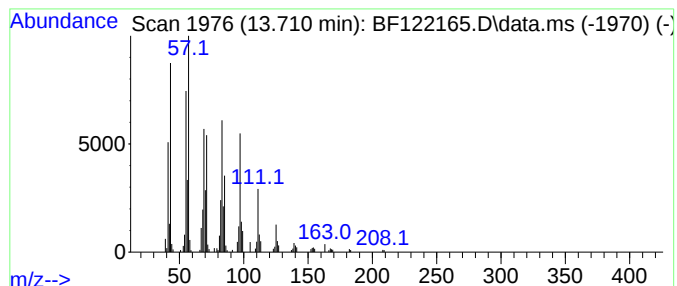
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	14.09 ng	688264	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3			Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	91
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5			17-Pentatriacontene	491	C35H70	006971-40-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102920\
Data File : BF122165.D
Acq On : 29 Oct 2020 15:40
Operator : JU/CG
Sample : L4547-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TT-033-IDWSO-20201027

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.210	16.2	ng	517751	1	6.710	637881	20.0
3-(2-Hydroxyeth...	9.269	6.7	ng	336952	3	9.745	1010450	20.0
n-Hexadecanoic ...	11.763	2.5	ng	130723	4	11.233	1041210	20.0
9-Octadecenamid...	13.292	3.5	ng	169177	5	13.880	977173	20.0
Heptadecyl trif...	13.710	14.1	ng	688264	5	13.880	977173	20.0
Hexaethylene gl...	14.174	2.4	ng	116564	5	13.880	977173	20.0