

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121621\
 Data File : BF126220.D
 Acq On : 16 Dec 2021 19:45
 Operator : JU/CG
 Sample : M4927-11
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PH1-BOT-12

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126220.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.869	299	303	308	rVB	61387	80334	1.83%	0.261%
2	5.022	490	499	507	rVB	638124	778850	17.75%	2.532%
3	5.422	562	567	571	rBV	3942052	4155356	94.72%	13.507%
4	6.439	734	740	744	rBV	3851007	4387108	100.00%	14.260%
5	6.816	800	804	807	rBV	1422570	1125493	25.65%	3.658%
6	7.375	894	899	902	rBV	3120822	2824105	64.37%	9.179%
7	7.998	1002	1005	1009	rBV	265135	196046	4.47%	0.637%
8	8.098	1018	1022	1025	rBV	1901331	1550237	35.34%	5.039%
9	9.175	1200	1205	1208	rBV	4721307	4189563	95.50%	13.618%
10	9.263	1217	1220	1223	rBV2	95987	87496	1.99%	0.284%
11	9.657	1282	1287	1294	rBV	127774	125437	2.86%	0.408%
12	9.851	1316	1320	1323	rBV	1892857	1531397	34.91%	4.978%
13	10.139	1361	1369	1373	rBV	30798	48839	1.11%	0.159%
14	10.263	1386	1390	1393	rBV2	96110	90744	2.07%	0.295%
15	10.633	1449	1453	1456	rBV	2258394	1987794	45.31%	6.461%
16	11.210	1544	1551	1553	rBV3	51309	61641	1.41%	0.200%
17	11.304	1563	1567	1569	rBV	100332	92682	2.11%	0.301%
18	11.333	1569	1572	1575	rVV	1601422	1281958	29.22%	4.167%
19	11.404	1579	1584	1586	rVB5	44396	55779	1.27%	0.181%
20	11.733	1637	1640	1643	rVB	93102	81621	1.86%	0.265%
21	12.321	1736	1740	1744	rBV3	37368	47739	1.09%	0.155%
22	12.921	1838	1842	1845	rBV	3464078	3088638	70.40%	10.039%
23	13.821	1991	1995	2004	rBV	477406	489975	11.17%	1.593%
24	13.968	2015	2020	2023	rBV	1190964	1066329	24.31%	3.466%
25	14.457	2100	2103	2108	rBV	104609	117605	2.68%	0.382%
26	15.092	2207	2211	2218	rBV2	63097	88620	2.02%	0.288%
27	15.409	2260	2265	2272	rBV2	717530	876736	19.98%	2.850%
28	15.898	2344	2348	2352	rBV	43402	59431	1.35%	0.193%
29	15.945	2352	2356	2363	rVV5	42287	75471	1.72%	0.245%
30	16.121	2382	2386	2393	rVB8	32713	64512	1.47%	0.210%
31	16.392	2429	2432	2440	rVB5	31619	58042	1.32%	0.189%

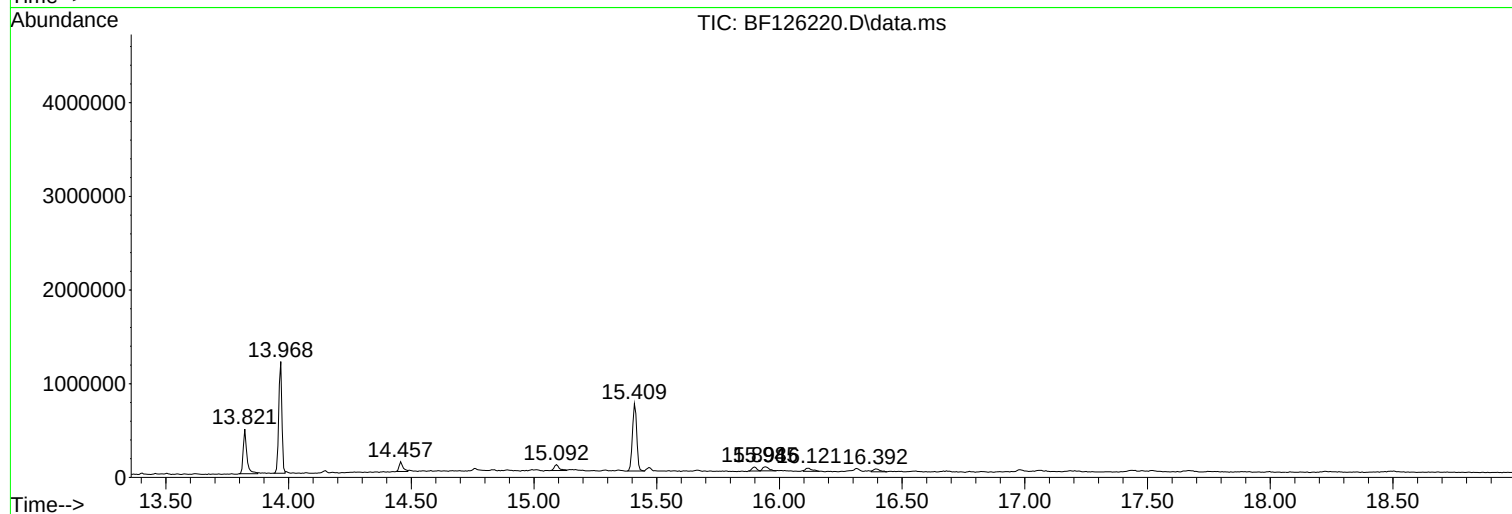
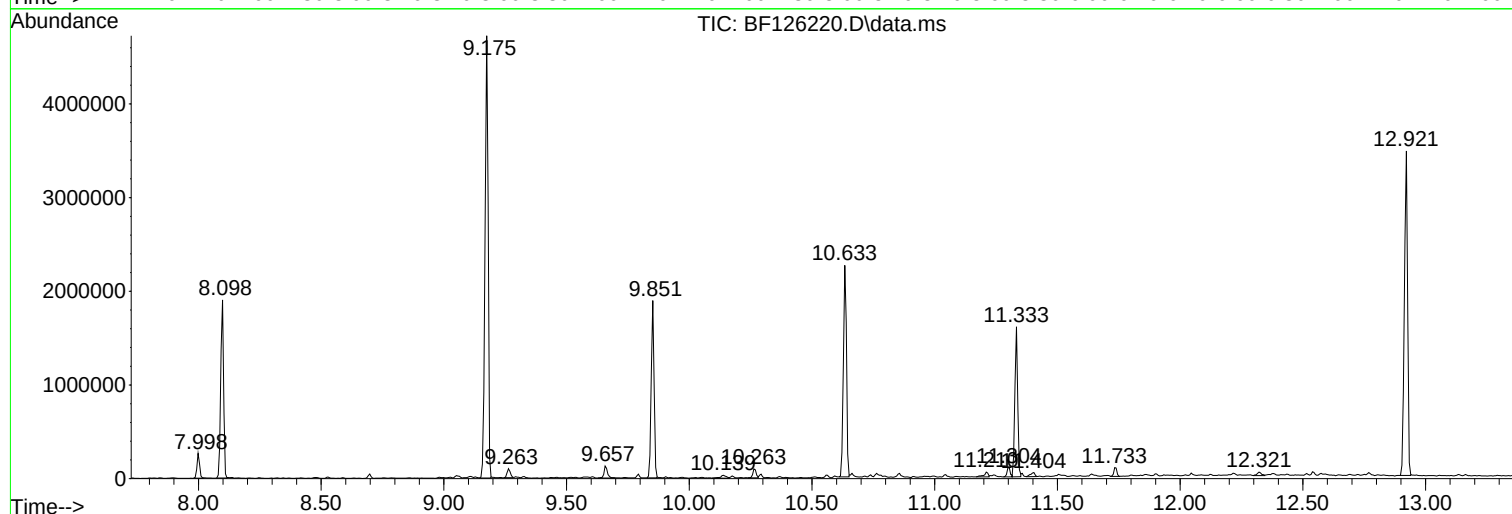
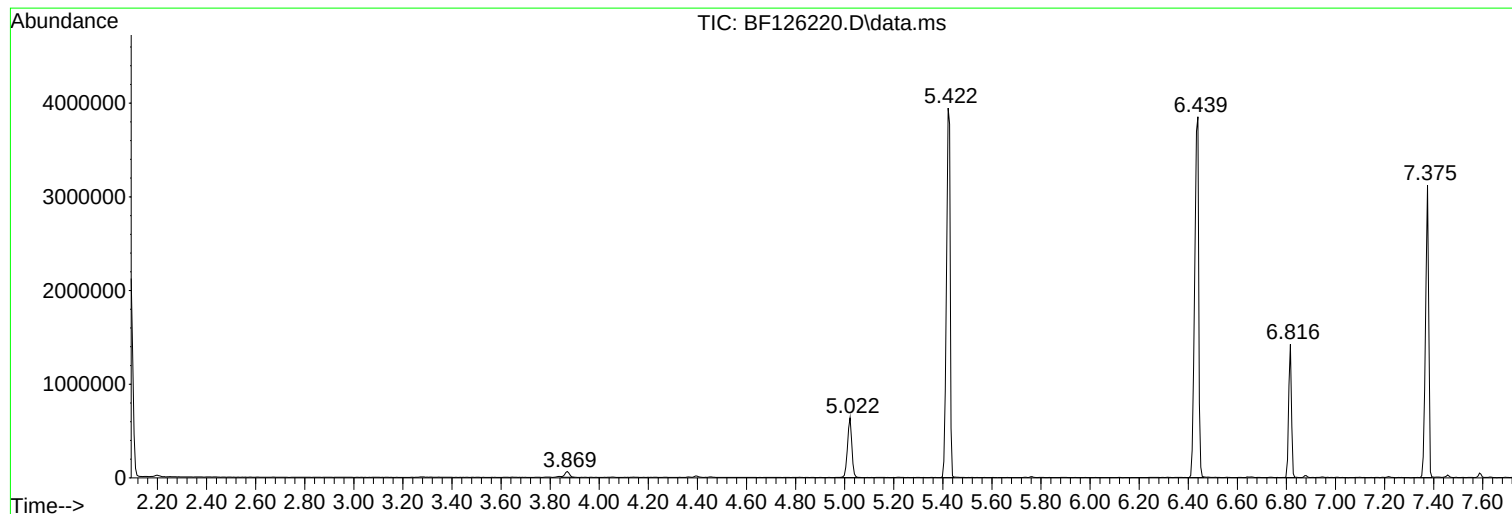
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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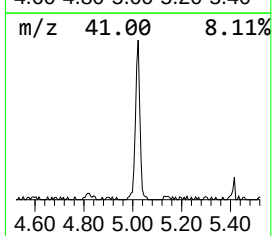
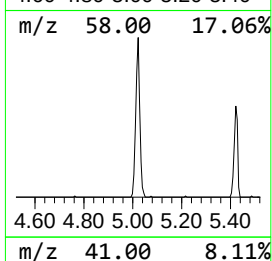
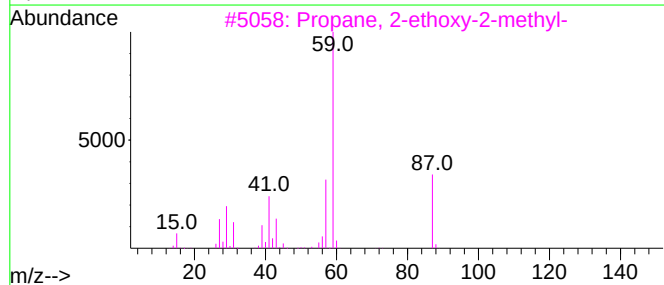
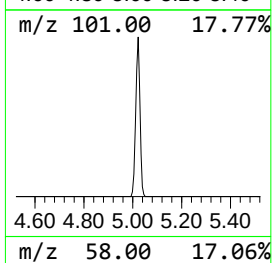
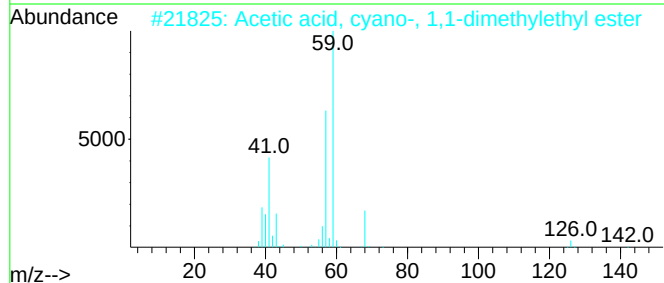
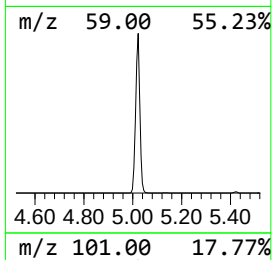
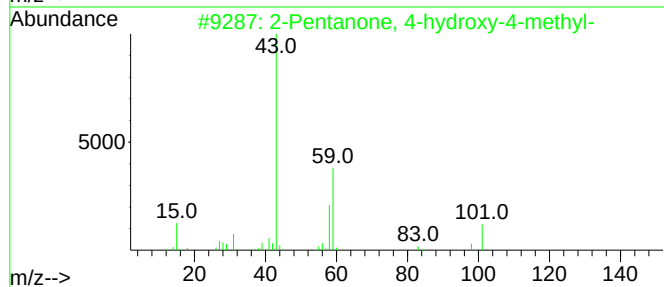
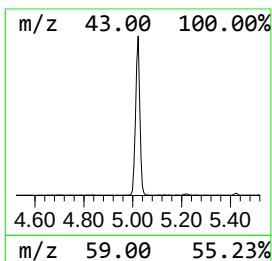
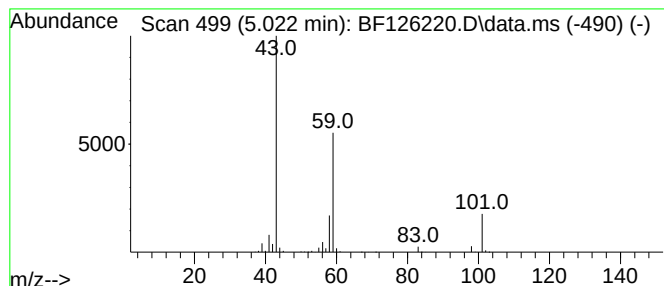
Instrument :
BNA_F
ClientSampleId :
PH1-BOT-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.022	13.84 ng	778850	1,4-Dichlorobenzene-d4	6.816	
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	23
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



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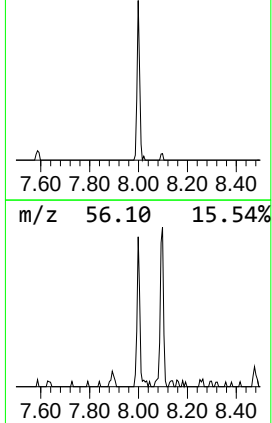
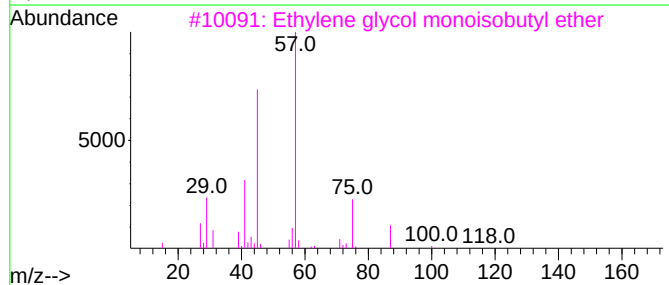
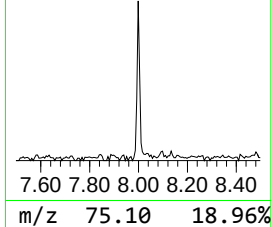
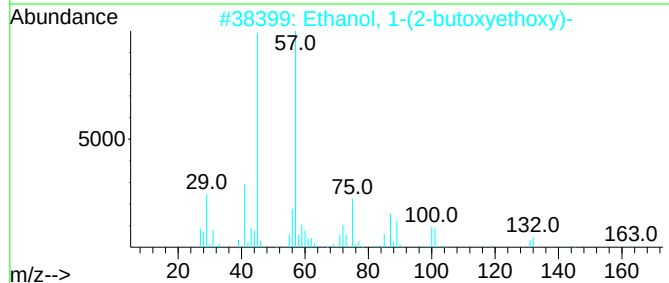
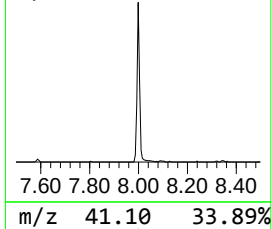
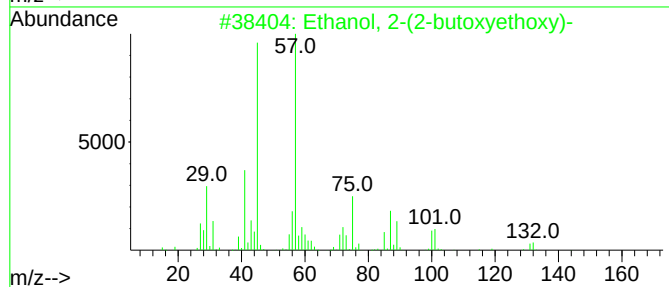
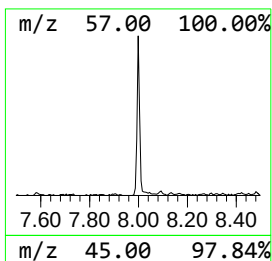
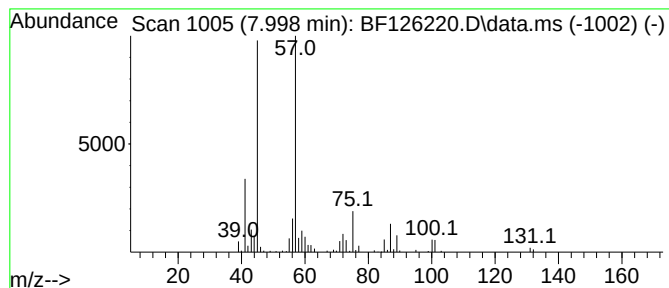
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.998	2.53 ng	196046	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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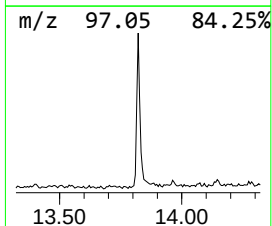
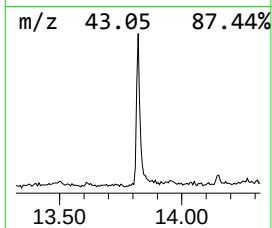
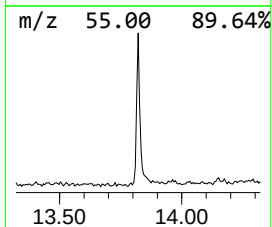
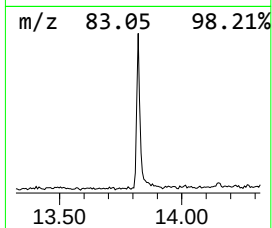
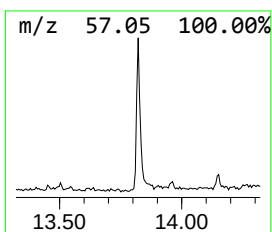
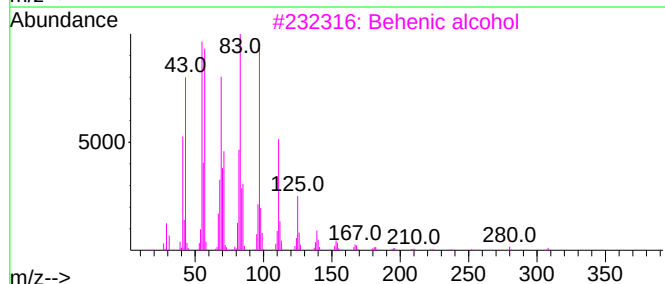
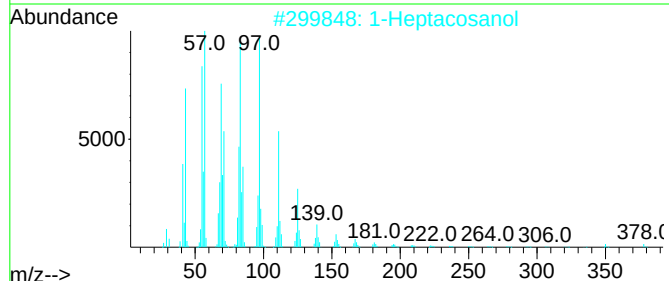
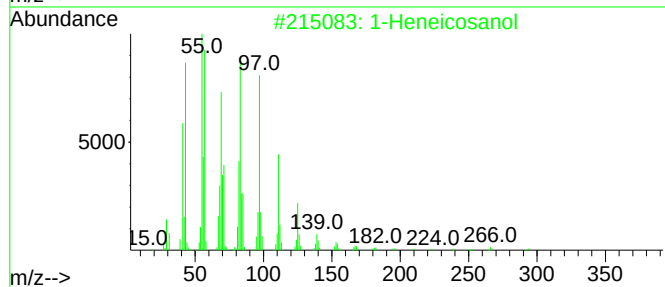
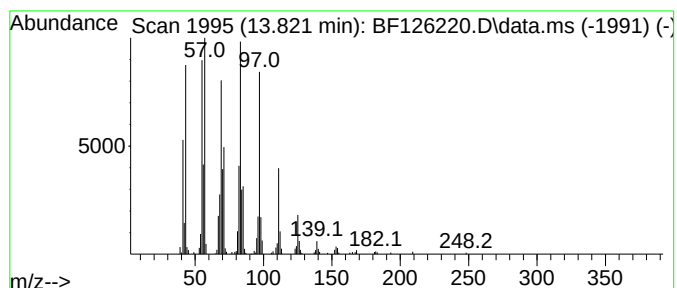
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	9.19 ng	489975	Chrysene-d12	13.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	94
2		1-Heptacosanol	396	C27H56O	002004-39-9	91
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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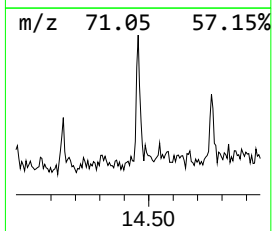
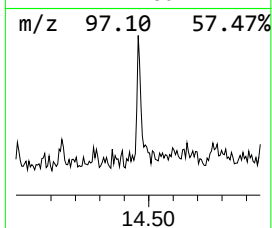
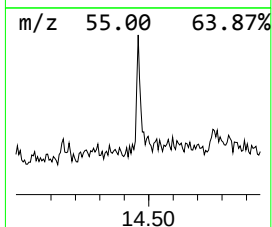
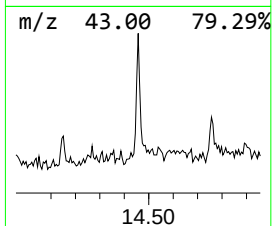
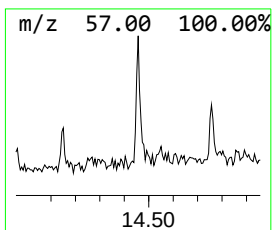
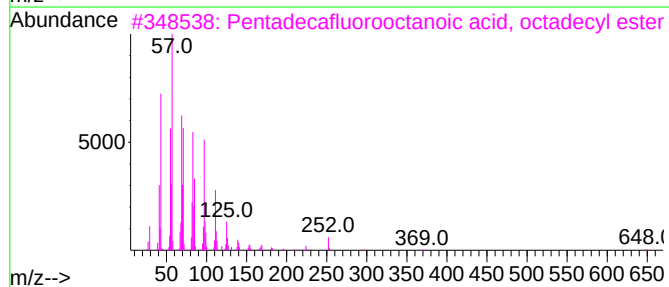
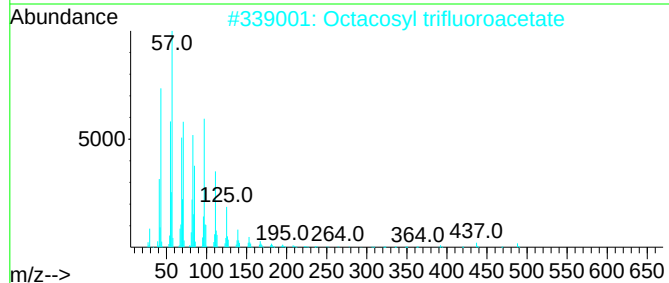
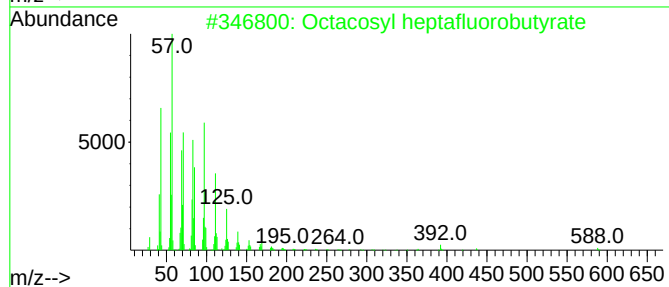
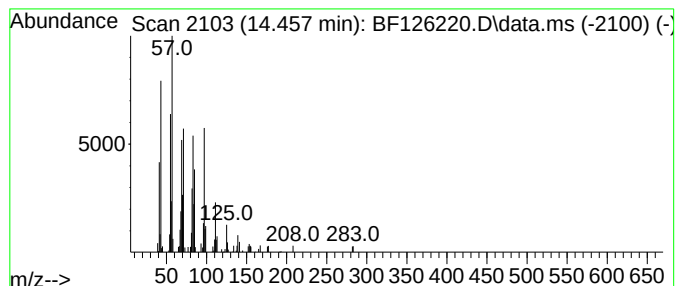
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octacosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	2.21 ng	117605	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
5			Butyl tetratriacontyl ether	551	C38H78O	1000406-41-4	91



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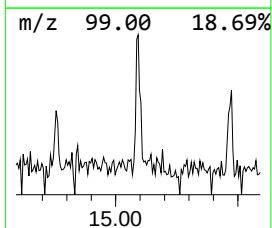
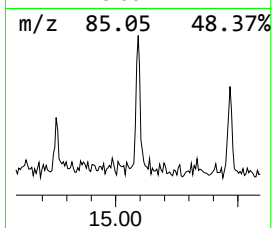
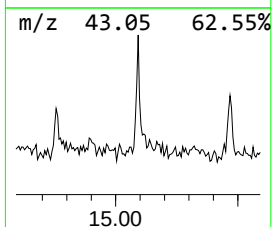
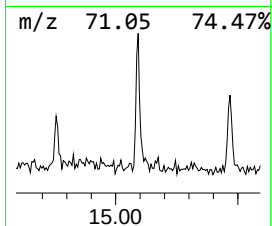
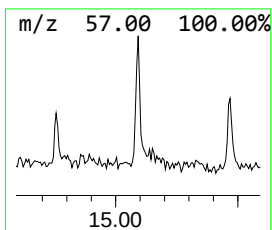
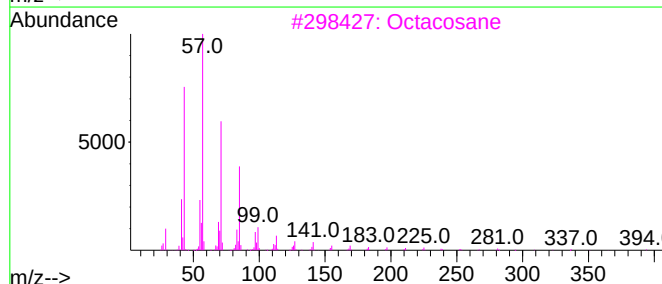
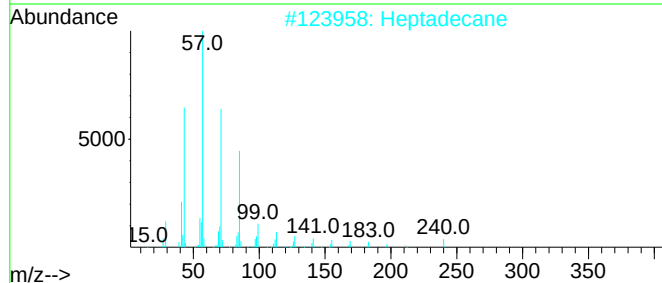
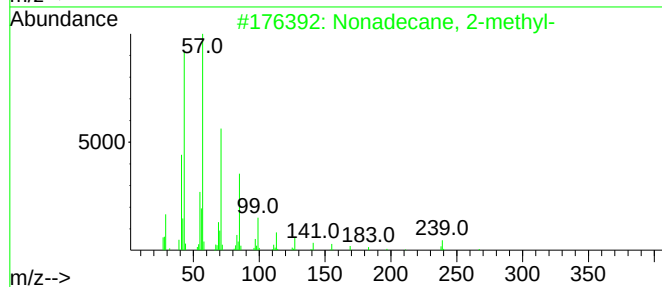
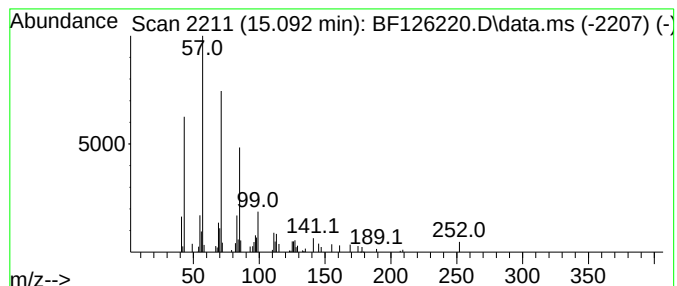
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonadecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.02 ng	88620	Perylene-d12	15.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
2		Heptadecane	240	C17H36	000629-78-7	86
3		Octacosane	394	C28H58	000630-02-4	86
4		Pentacosane	352	C25H52	000629-99-2	83
5		Heneicosane	296	C21H44	000629-94-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	13.8	ng	778850	1	6.816	1125490	20.0
Ethanol, 2-(2-b...	7.998	2.5	ng	196046	2	8.098	1550240	20.0
1-Heneicosanol	13.821	9.2	ng	489975	5	13.968	1066330	20.0
Octacosyl hepta...	14.457	2.2	ng	117605	5	13.968	1066330	20.0
Nonadecane, 2-m...	15.092	2.0	ng	88620	6	15.410	876736	20.0