

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
 Data File : BF137824.D
 Acq On : 02 May 2024 19:56
 Operator : CG\JU
 Sample : P2331-16
 Misc :
 ALS Vial : 22 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-BF043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	16	20	27	rVB2	64775	110757	2.88%	0.436%
2	2.428	51	58	65	rVB	1603749	2092160	54.45%	8.236%
3	3.693	271	273	286	rBV	49848	85621	2.23%	0.337%
4	5.304	543	547	551	rVB	40799	45415	1.18%	0.179%
5	5.681	606	611	614	rBV	4042225	3842333	100.00%	15.126%
6	6.669	773	779	782	rBV	2393946	2517676	65.52%	9.911%
7	7.057	841	845	848	rBV	961930	813964	21.18%	3.204%
8	7.616	935	940	943	rBV	1652772	1485309	38.66%	5.847%
9	8.339	1059	1063	1066	rBV	1401759	1107707	28.83%	4.361%
10	8.639	1111	1114	1124	rBV	43076	54202	1.41%	0.213%
11	9.410	1241	1245	1249	rBV	3296584	2960124	77.04%	11.653%
12	10.098	1358	1362	1366	rBV	1465350	1291758	33.62%	5.085%
13	10.181	1372	1376	1385	rVB	51407	71513	1.86%	0.282%
14	10.892	1492	1497	1500	rBV	2240509	1959071	50.99%	7.712%
15	11.592	1613	1616	1620	rBV	1381577	1216755	31.67%	4.790%
16	12.098	1699	1702	1712	rBV	293394	302250	7.87%	1.190%
17	12.886	1833	1836	1846	rBV	120430	128154	3.34%	0.504%
18	13.180	1882	1886	1890	rBV	2969430	2531207	65.88%	9.964%
19	14.110	2039	2044	2053	rBV5	35871	115305	3.00%	0.454%
20	14.245	2063	2067	2071	rBV	1193318	1044529	27.18%	4.112%
21	14.386	2087	2091	2094	rBV	51536	47215	1.23%	0.186%
22	14.692	2140	2143	2148	rVB	57813	57453	1.50%	0.226%
23	15.027	2197	2200	2206	rVB	41043	43481	1.13%	0.171%
24	15.115	2211	2215	2220	rVV2	37600	43340	1.13%	0.171%
25	15.192	2224	2228	2233	rVB	60613	71340	1.86%	0.281%
26	15.398	2259	2263	2270	rVB	54508	61782	1.61%	0.243%
27	15.815	2328	2334	2342	rBV	845952	1111802	28.94%	4.377%
28	16.051	2369	2374	2380	rBV2	76419	113626	2.96%	0.447%
29	16.310	2414	2418	2424	rVB2	49336	76452	1.99%	0.301%

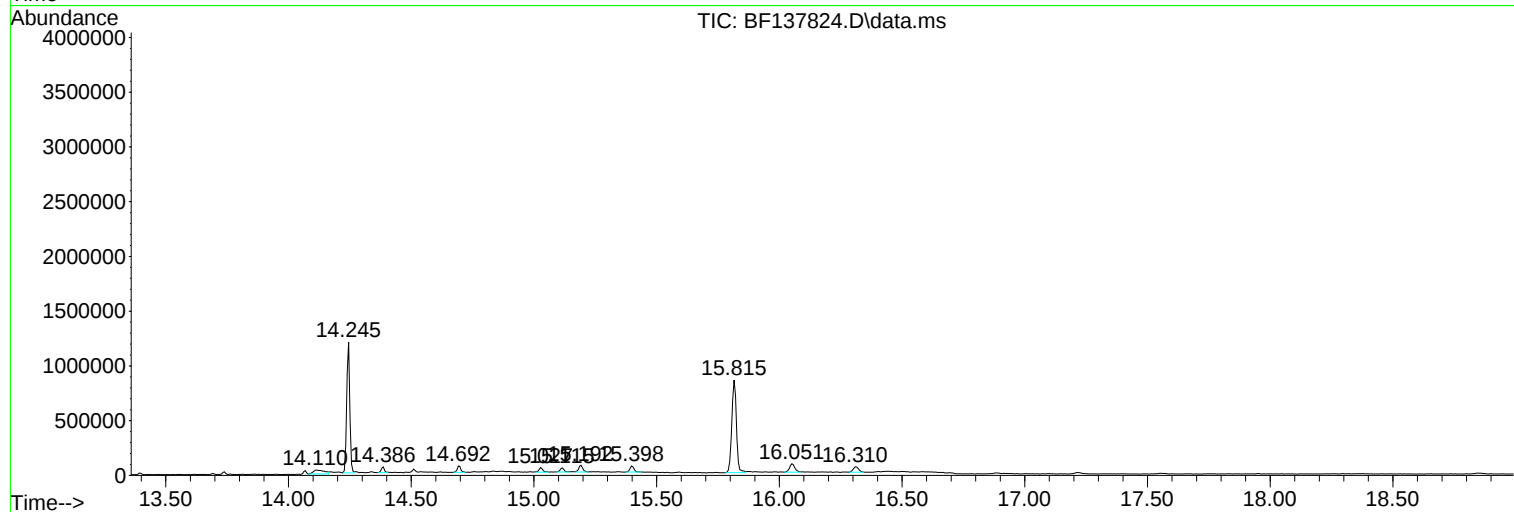
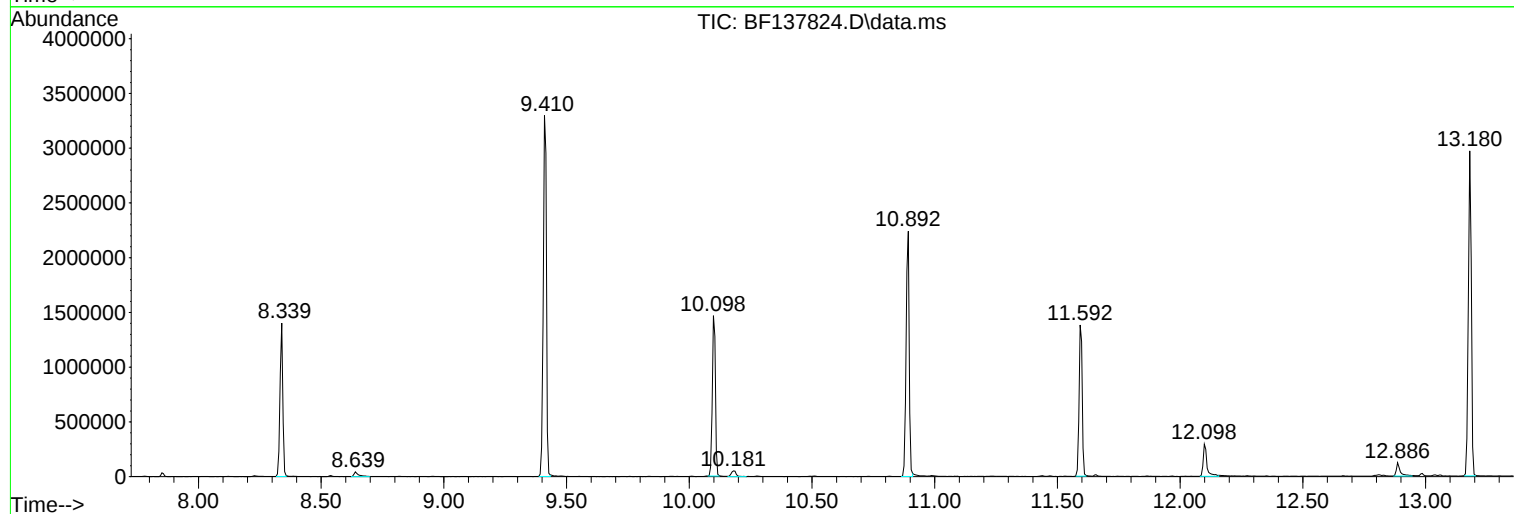
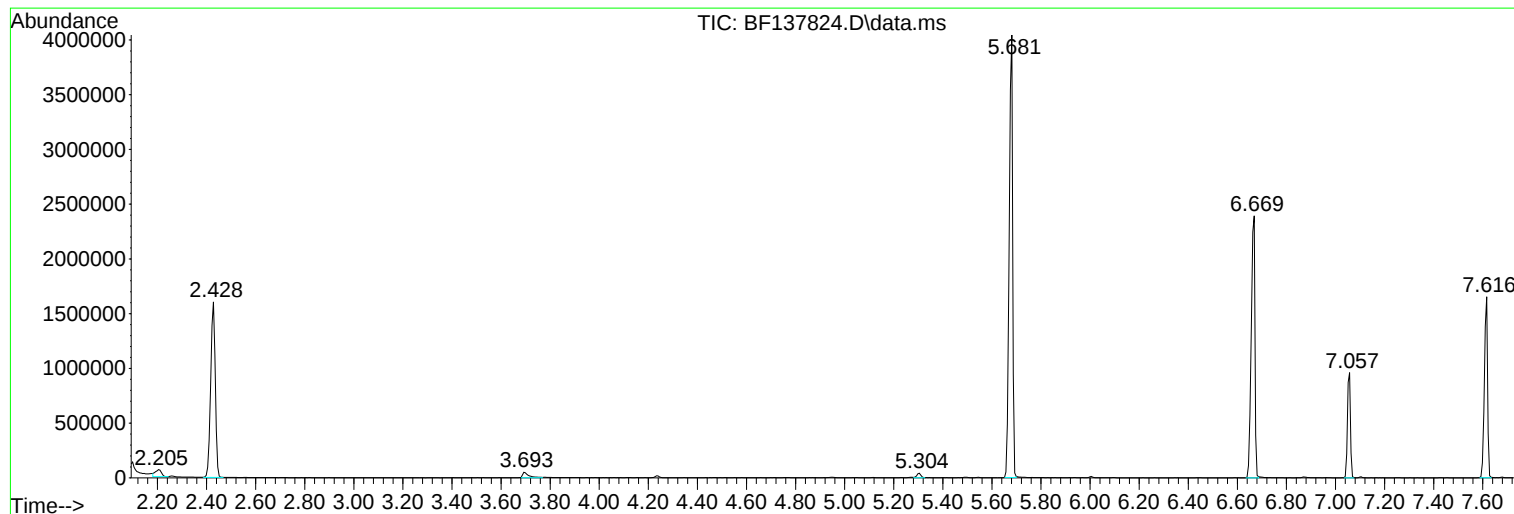
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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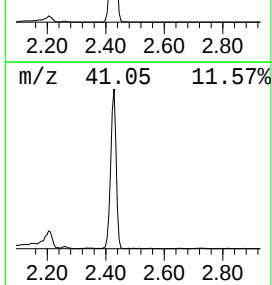
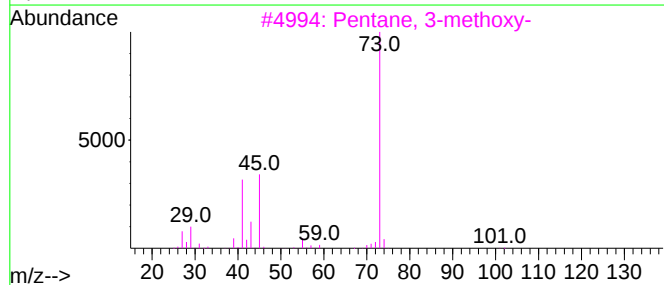
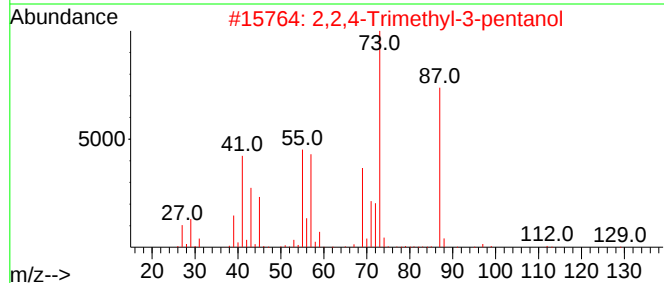
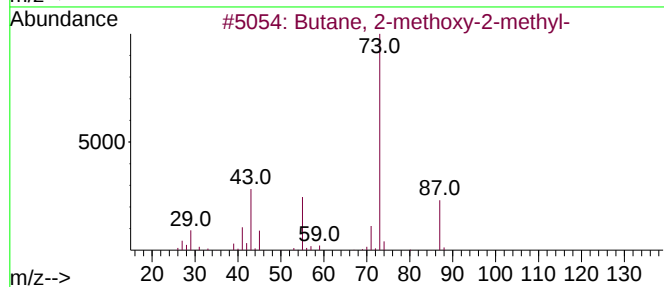
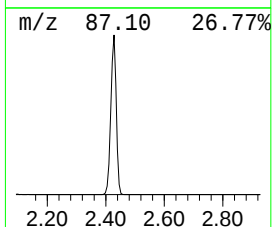
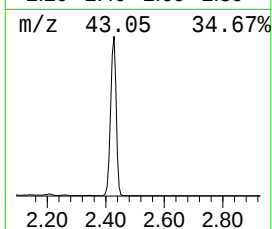
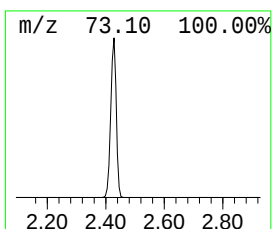
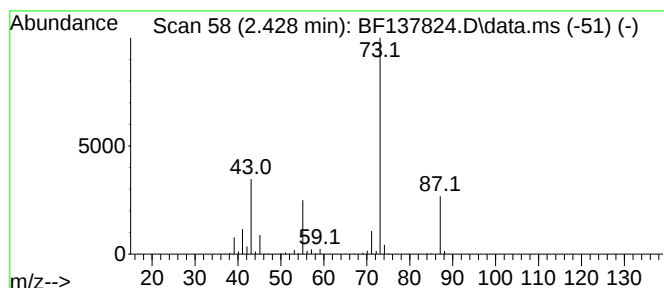
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.428	51.41 ng	2092160	1,4-Dichlorobenzene-d4	7.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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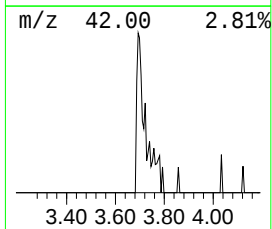
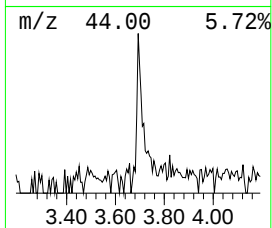
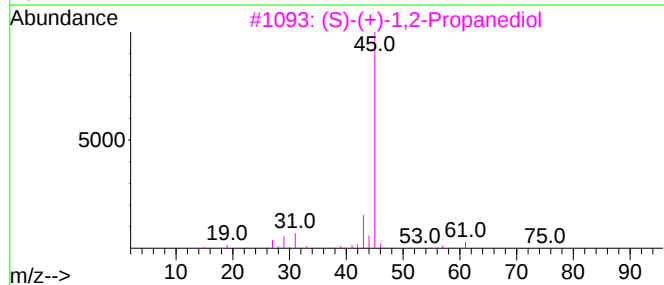
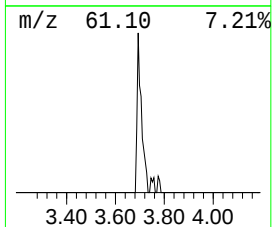
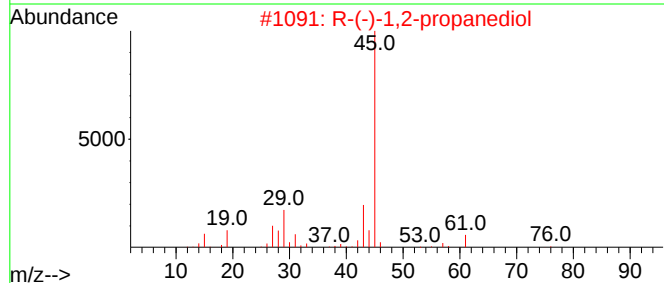
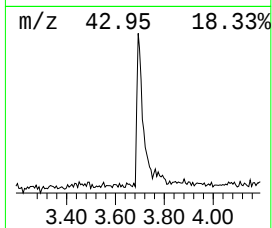
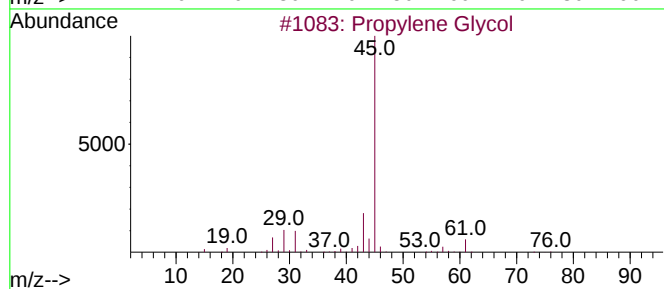
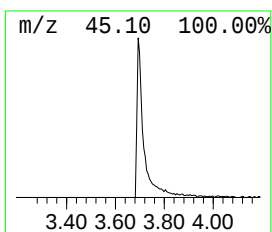
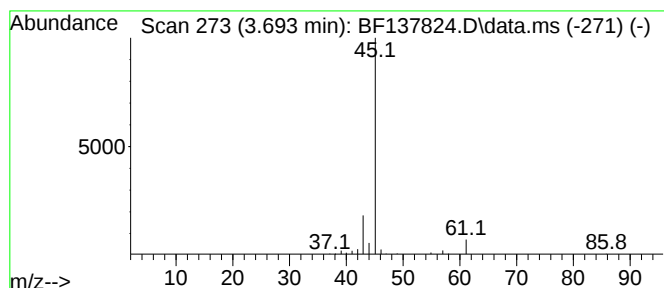
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown3.693 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.693	2.10 ng	85621	1,4-Dichlorobenzene-d4	7.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propylene Glycol	76	C3H8O2	000057-55-6	43
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4		1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9
5		2-Pentanol	88	C5H12O	006032-29-7	9



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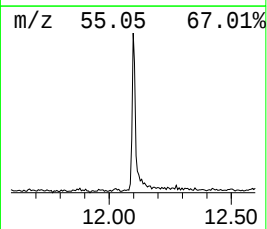
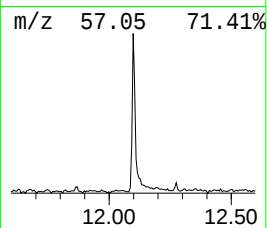
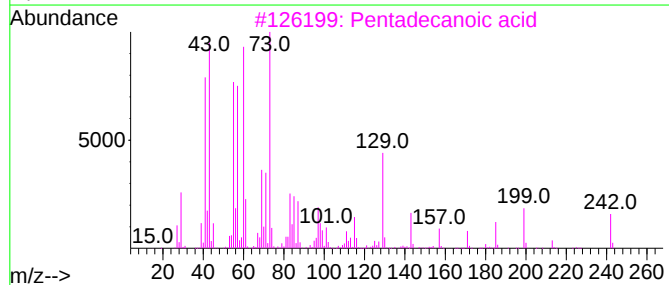
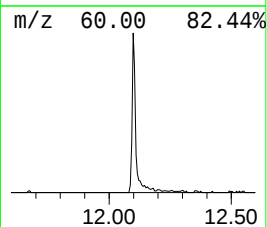
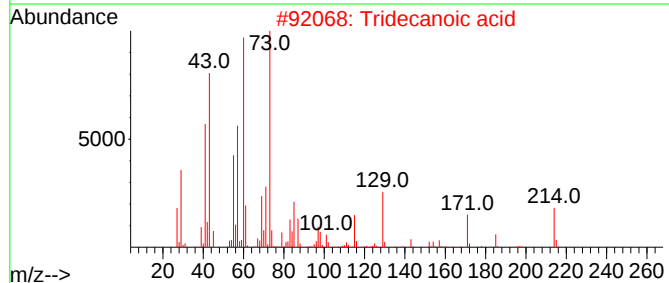
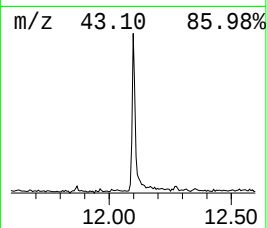
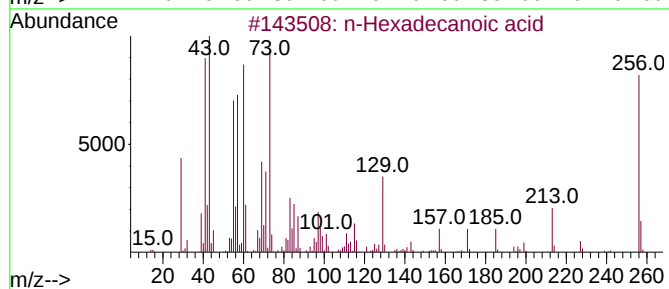
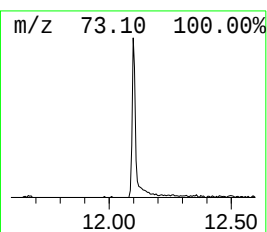
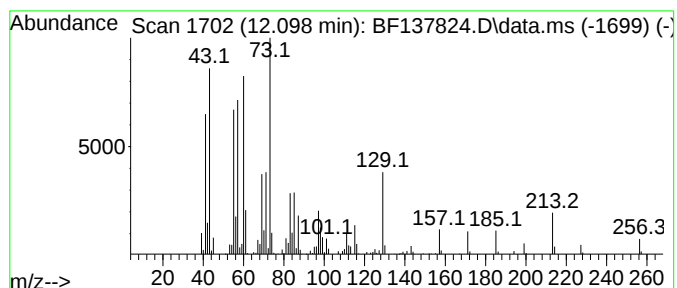
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.098	4.97 ng	302250	Phenanthrene-d10		11.592	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tridecanoic acid		214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	81
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	70



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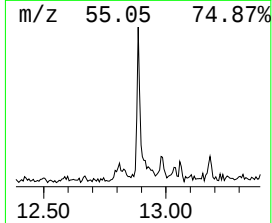
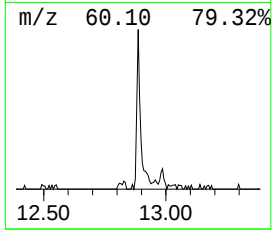
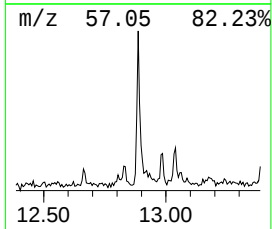
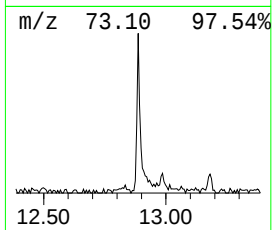
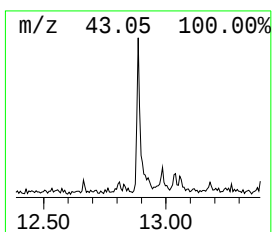
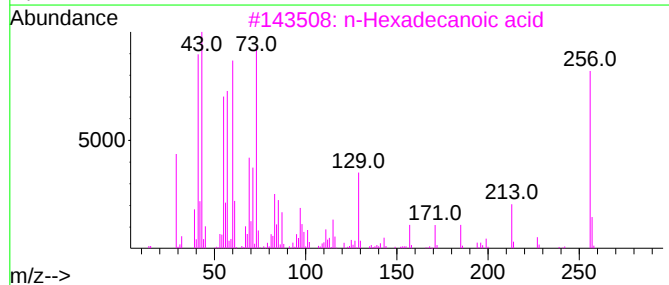
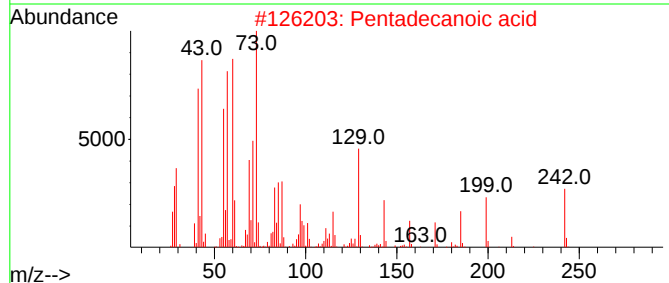
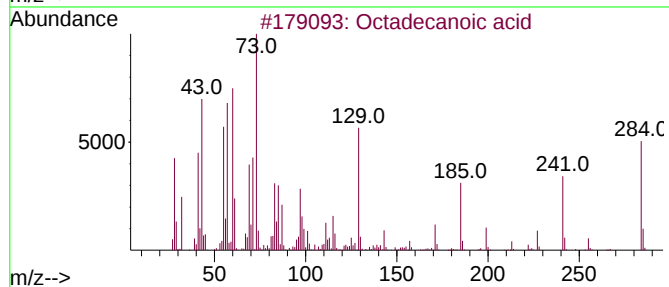
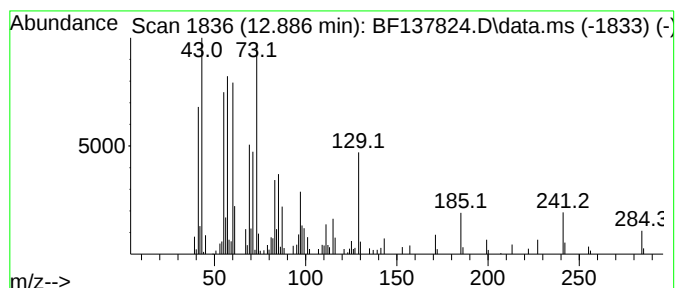
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	2.11 ng	128154	Phenanthrene-d10	11.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	43



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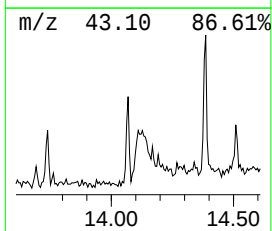
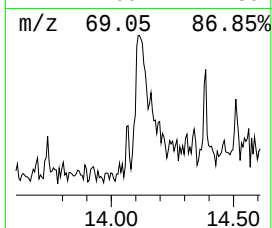
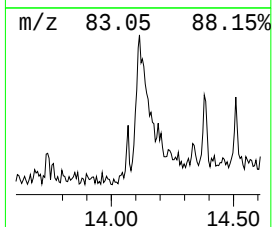
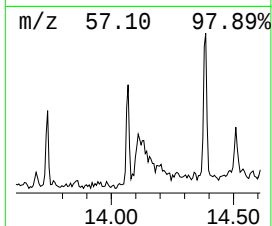
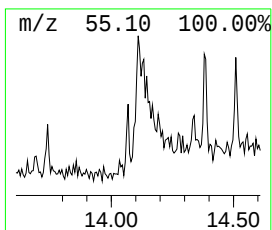
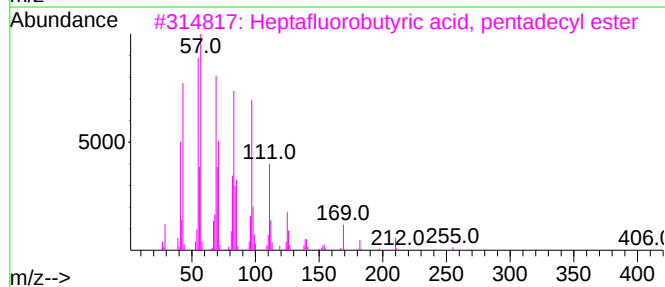
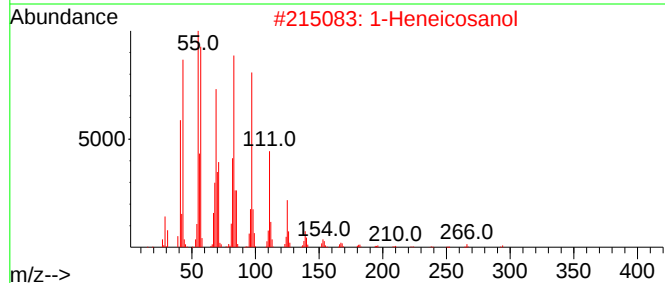
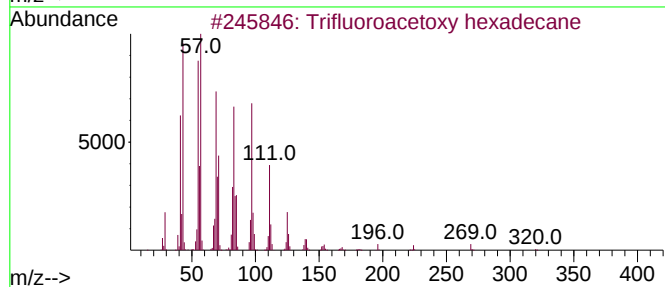
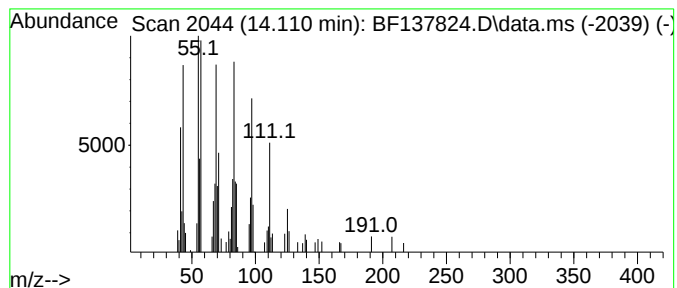
Instrument :
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.110	2.21 ng	115305	Chrysene-d12		14.245	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
2	1-Heneicosanol		312	C21H44O	015594-90-8	91
3	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	91
4	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2	959010-23-2	91
5	1-Hexadecanol		242	C16H34O	036653-82-4	91



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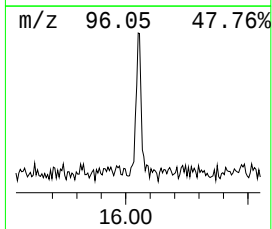
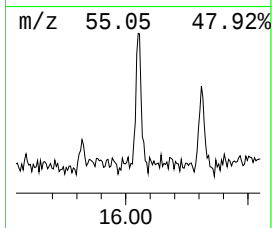
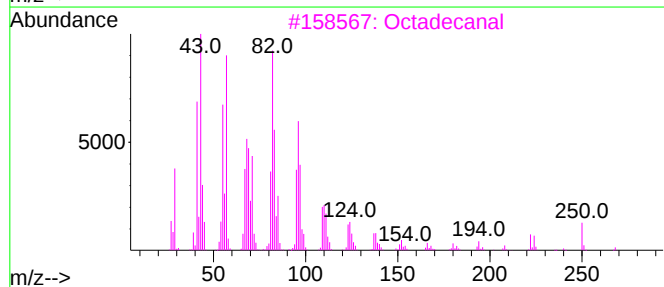
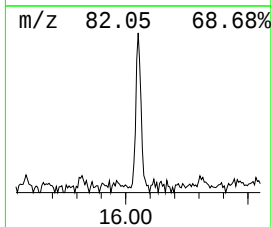
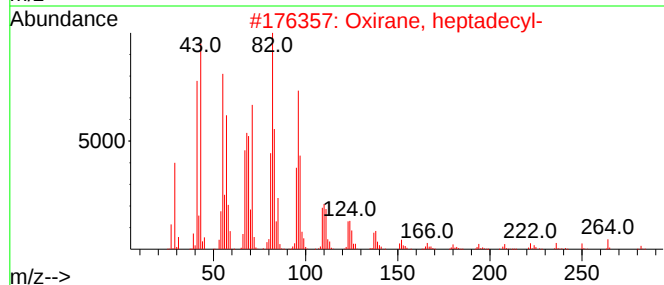
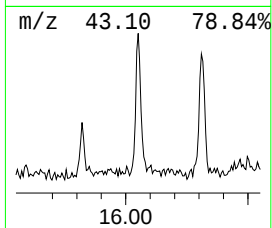
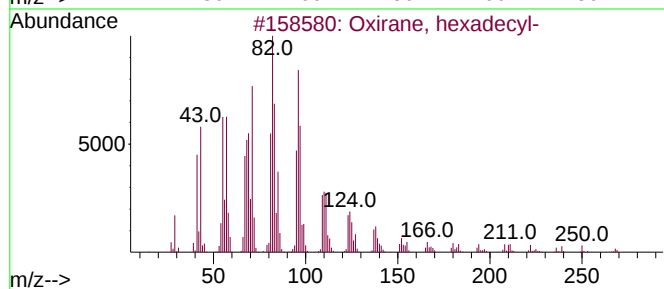
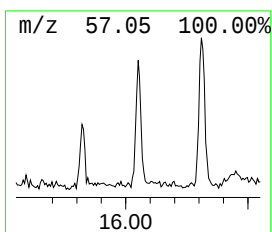
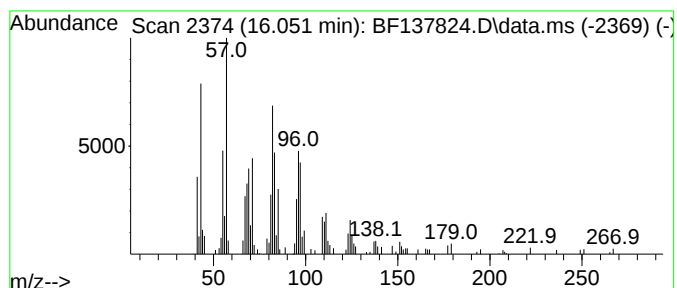
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.051	2.04 ng	113626	Perylene-d12	15.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
3			Octadecanal	268	C18H36O	000638-66-4	64
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	49
5			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137824.D
Acq On : 02 May 2024 19:56
Operator : CG\JU
Sample : P2331-16
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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...	2.428	51.4	ng	2092160	1	7.057	813964	20.0
unknown3.693	3.693	2.1	ng	85621	1	7.057	813964	20.0
n-Hexadecanoic ...	12.098	5.0	ng	302250	4	11.592	1216760	20.0
Octadecanoic acid	12.886	2.1	ng	128154	4	11.592	1216760	20.0
Trifluoroacetox...	14.110	2.2	ng	115305	5	14.245	1044530	20.0
Oxirane, hexade...	16.051	2.0	ng	113626	6	15.815	1111800	20.0