

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
 Data File : BF139029.D
 Acq On : 15 Aug 2024 18:40
 Operator : RC/JU
 Sample : P3580-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 923-K1-SD-0-0.5-081224

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-BF073024.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.428	223	227	235	rBV2	2791	8912	1.15%	0.162%
2	5.057	500	504	519	rVB	27872	43591	5.60%	0.793%
3	5.316	544	548	554	rBB	6768	8461	1.09%	0.154%
4	5.469	569	574	593	rBV	502052	713397	91.66%	12.980%
5	6.481	741	746	771	rBV	563609	778301	100.00%	14.161%
6	6.834	802	806	812	rBV	191233	231429	29.74%	4.211%
7	7.398	897	902	916	rBV	350162	455625	58.54%	8.290%
8	7.663	943	947	955	rBB	8036	13389	1.72%	0.244%
9	8.116	1019	1024	1045	rVB	242339	302369	38.85%	5.502%
10	8.434	1074	1078	1090	rBV	29088	45012	5.78%	0.819%
11	9.186	1201	1206	1215	rBV	542504	664901	85.43%	12.098%
12	9.863	1316	1321	1330	rBV	266726	344745	44.29%	6.273%
13	9.957	1332	1337	1343	rVV	17340	24631	3.16%	0.448%
14	10.657	1451	1456	1467	rBV	346849	452598	58.15%	8.235%
15	11.357	1569	1575	1586	rBV	251802	336485	43.23%	6.122%
16	11.874	1659	1663	1671	rBV6	7371	14759	1.90%	0.269%
17	12.574	1778	1782	1787	rVB	12139	13990	1.80%	0.255%
18	12.804	1815	1821	1828	rBV	9887	14876	1.91%	0.271%
19	12.933	1838	1843	1848	rBV	340184	413766	53.16%	7.529%
20	13.827	1988	1995	2001	rBV4	13899	38343	4.93%	0.698%
21	13.886	2001	2005	2009	rVB	41768	51575	6.63%	0.938%
22	13.998	2019	2024	2034	rVB	140490	193155	24.82%	3.514%
23	14.439	2095	2099	2103	rBV2	10748	16062	2.06%	0.292%
24	14.515	2109	2112	2117	rVB	9903	11922	1.53%	0.217%
25	15.074	2203	2207	2212	rVB	39197	54501	7.00%	0.992%
26	15.462	2267	2273	2282	rVB	123521	189855	24.39%	3.454%
27	15.645	2301	2304	2311	rVB5	6553	9905	1.27%	0.180%
28	15.874	2337	2343	2349	rVB	16744	28211	3.62%	0.513%
29	16.368	2423	2427	2435	rVB8	4316	8613	1.11%	0.157%
30	16.657	2471	2476	2481	rBV5	6583	12582	1.62%	0.229%

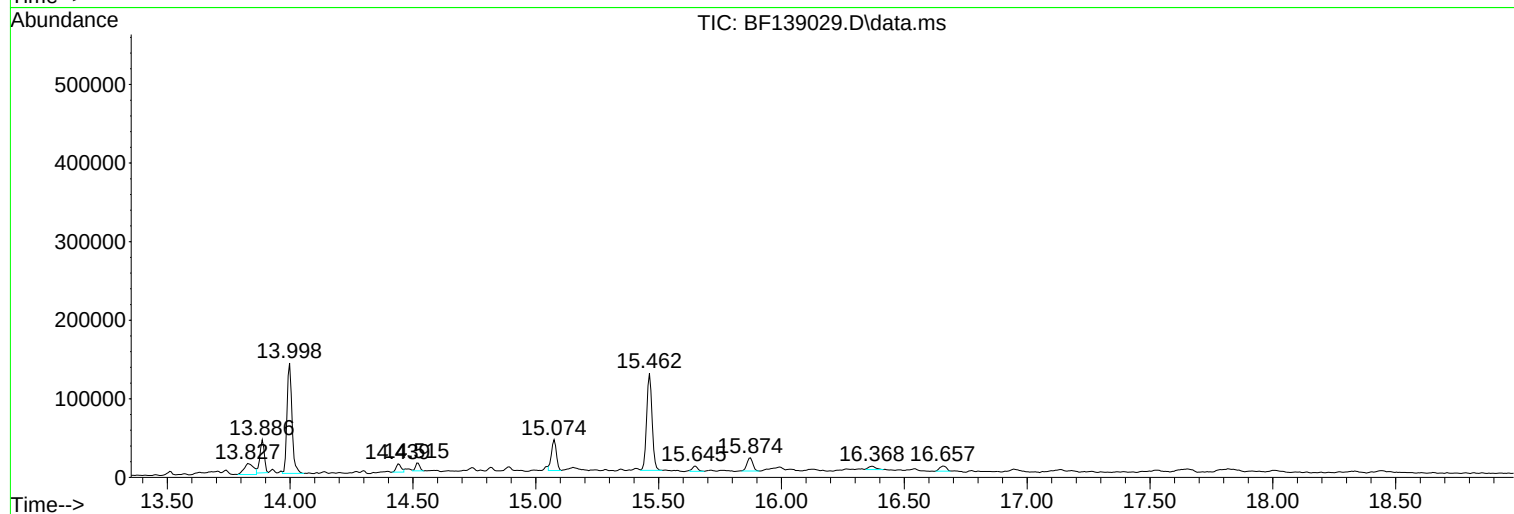
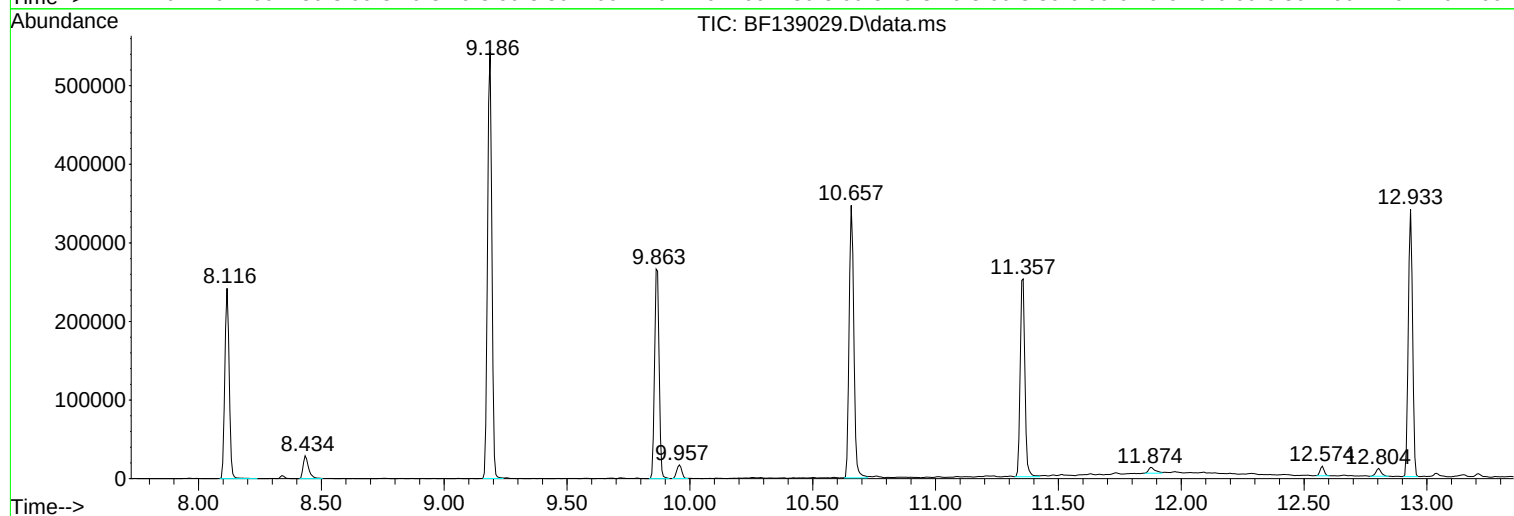
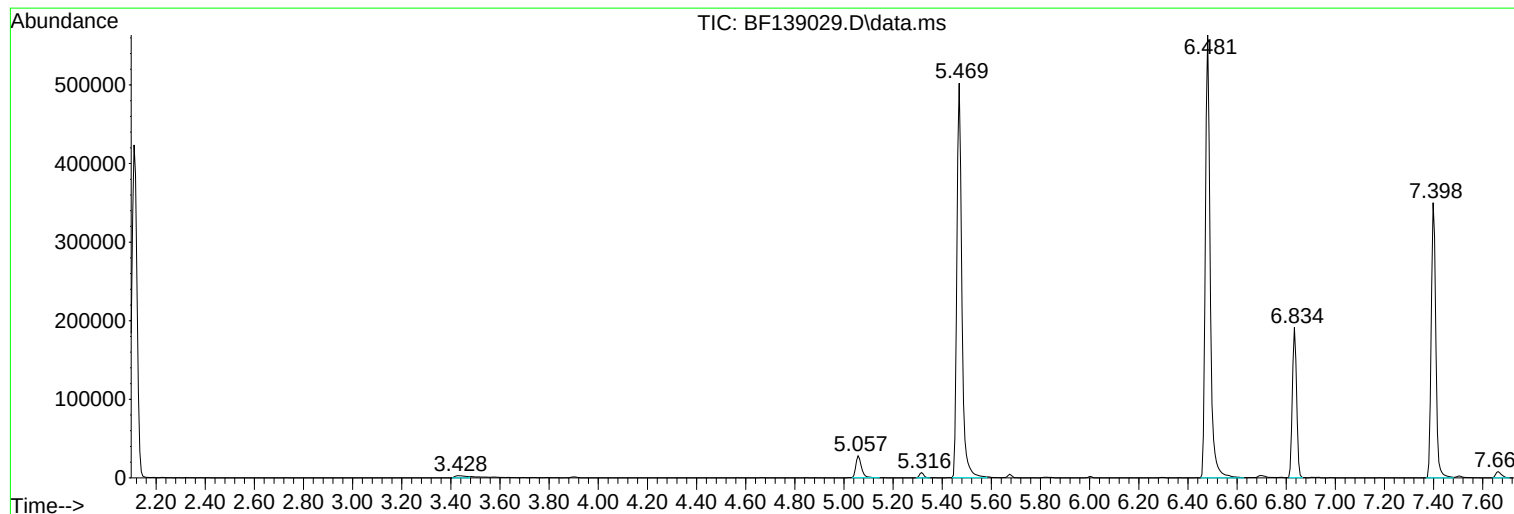
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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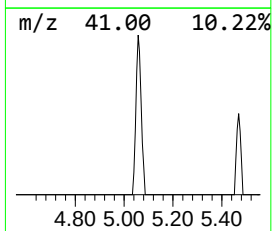
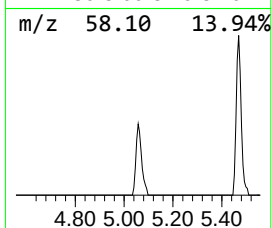
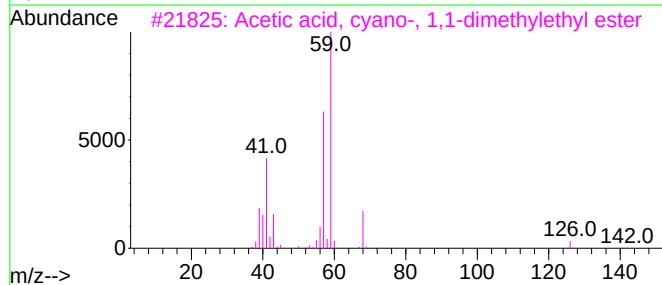
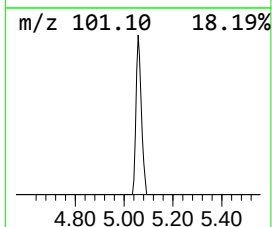
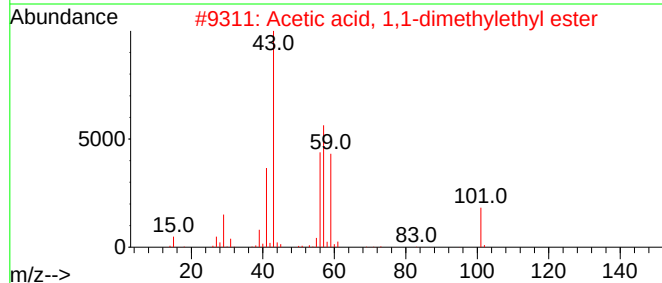
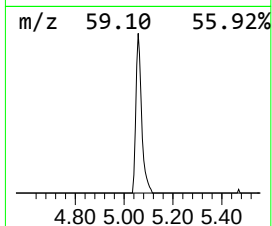
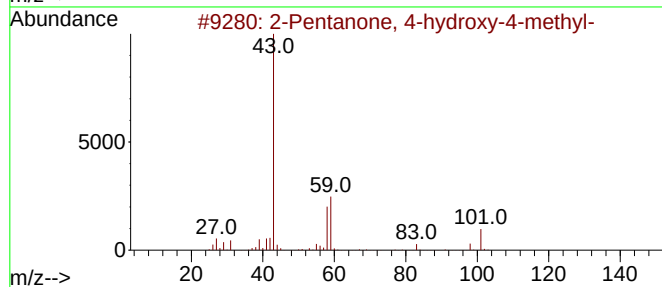
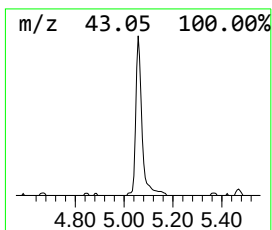
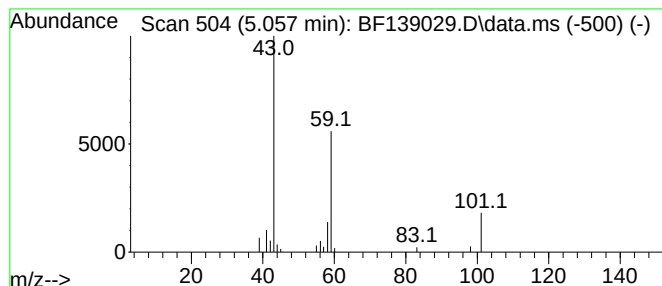
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	3.77 ng	43591	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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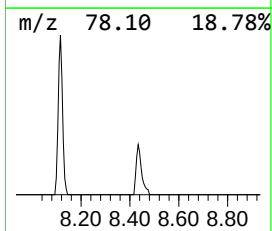
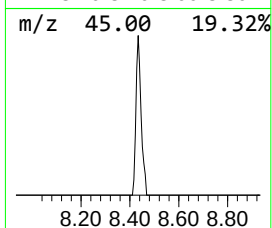
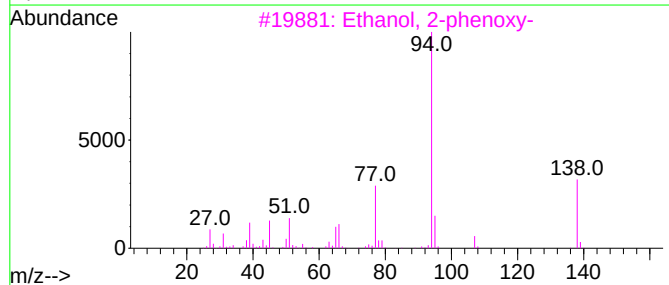
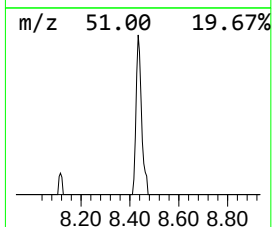
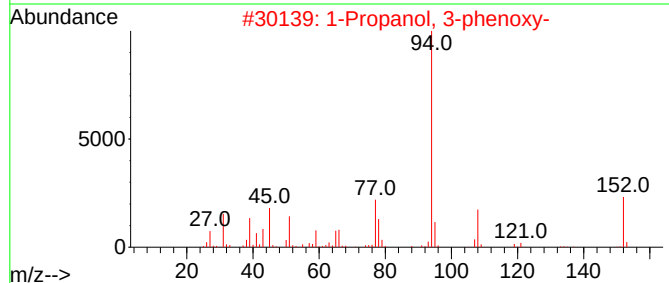
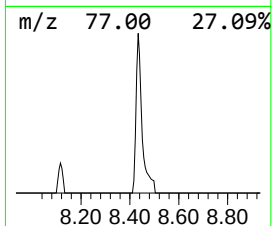
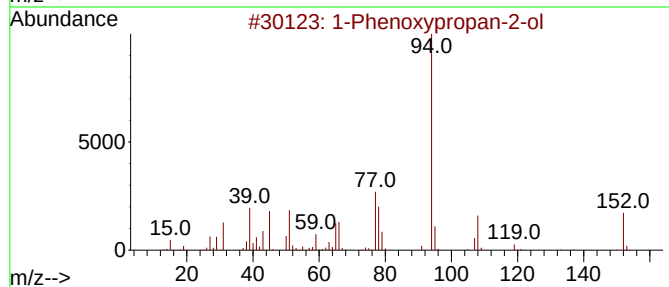
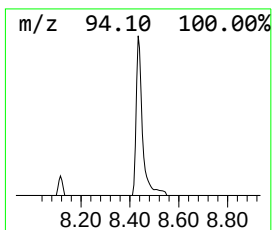
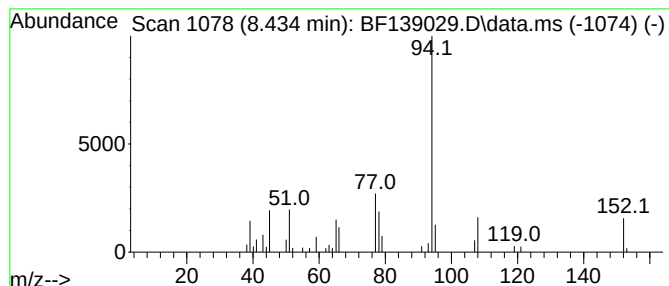
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	2.98 ng	45012	Naphthalene-d8	8.116

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	91
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	53
5			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53



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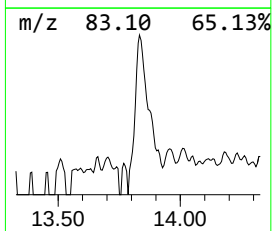
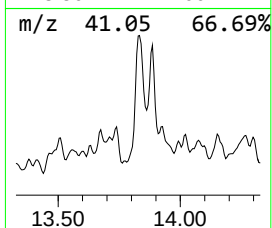
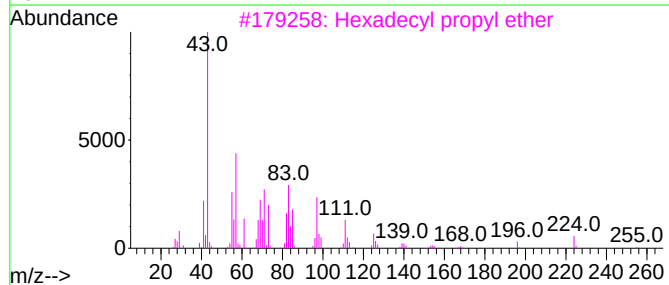
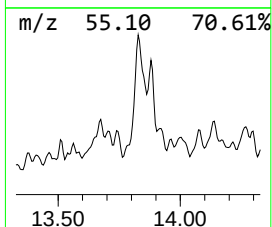
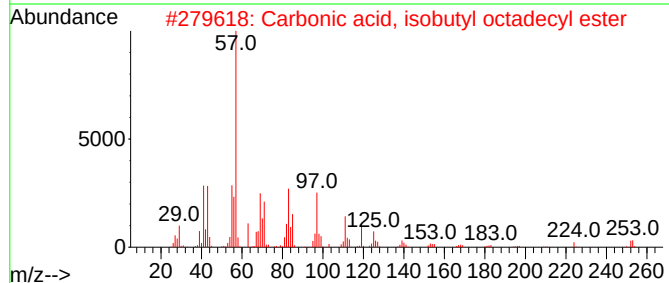
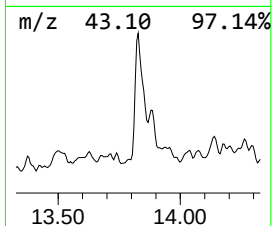
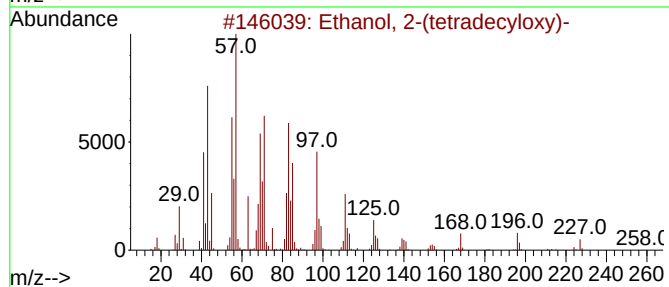
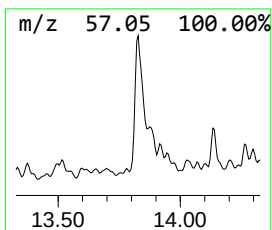
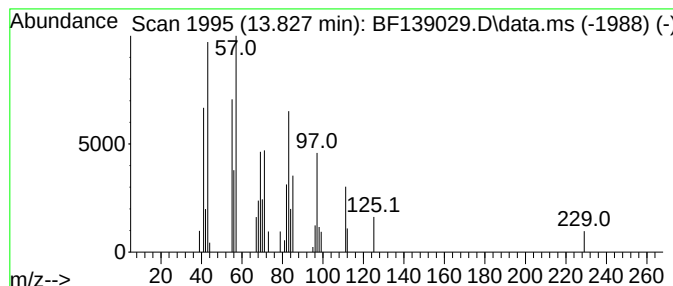
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	3.97 ng	38343	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91
3			Hexadecyl propyl ether	284	C19H40O	1000406-27-9	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Octacosyl propyl ether	452	C31H64O	1000406-28-5	87



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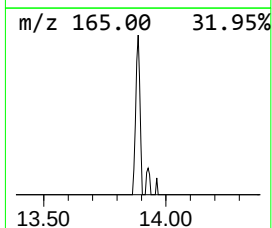
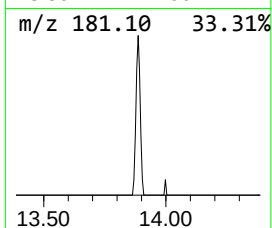
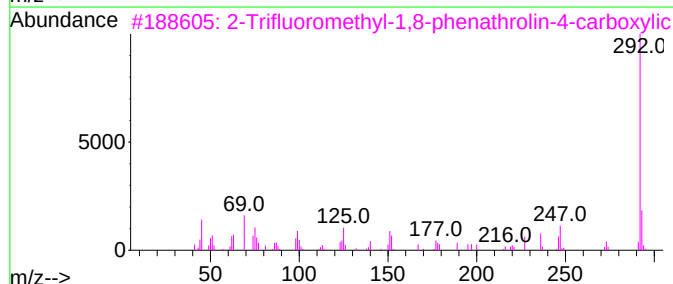
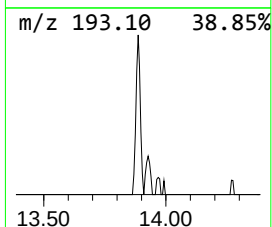
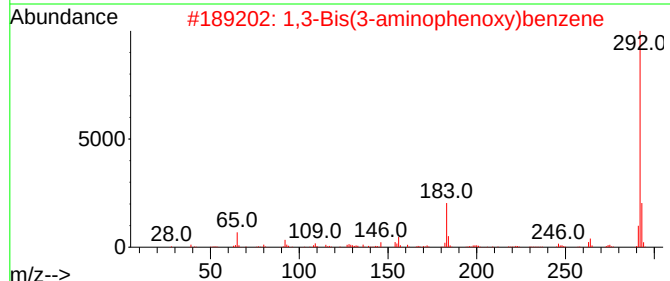
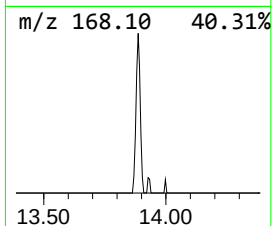
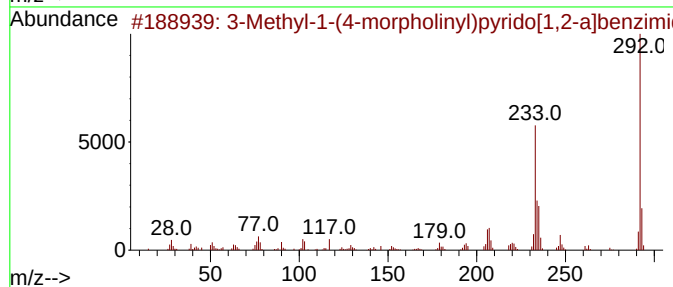
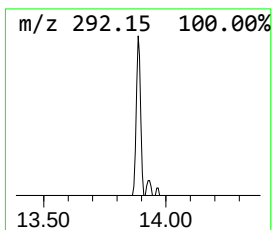
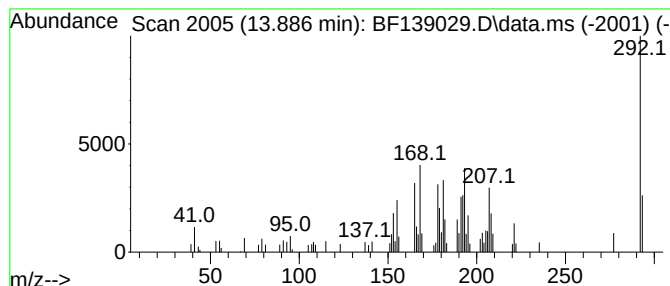
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Peak Number 4 unknown13.886 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	5.34 ng	51575	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-1-(4-morpholinyl)pyrido...	292	C17H16N4O	1000331-84-7	25
2			1,3-Bis(3-aminophenoxy)benzene	292	C18H16N2O2	010526-07-5	22
3			2-Trifluoromethyl-1,8-phenathrol...	292	C14H7F3N2O2	050509-89-2	22
4			2-(4-Fluorophenyl)-5-methoxy-2H-...	292	C18H13FN2O	1000194-51-1	22
5			(O-Decylphenoxy)acetic acid	292	C18H28O3	014353-81-2	22



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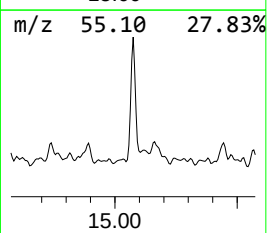
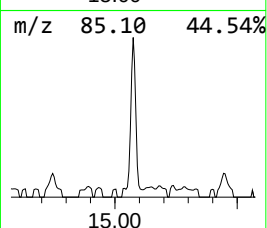
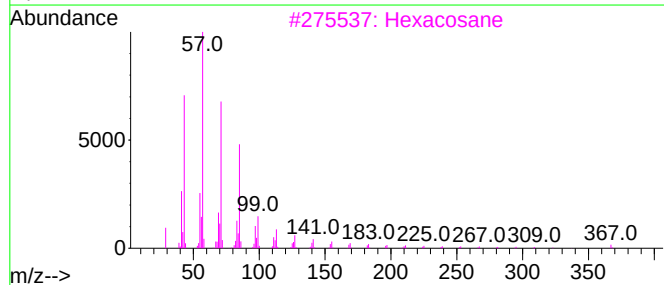
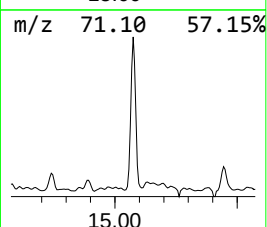
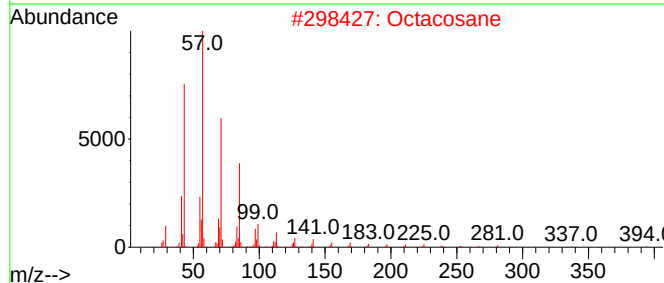
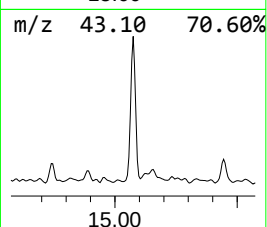
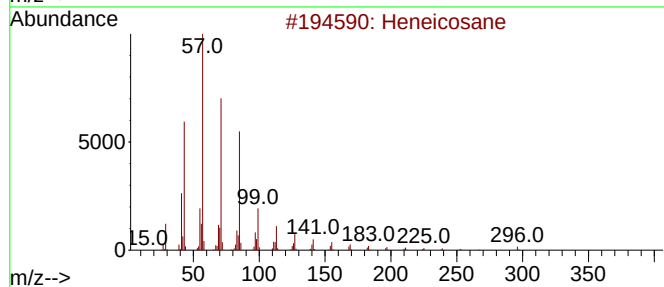
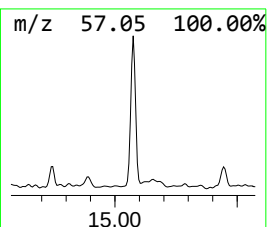
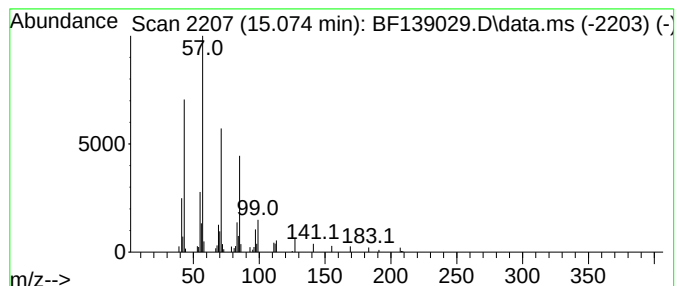
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Peak Number 5 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	5.74 ng	54501	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Tetracosane	338	C24H50	000646-31-1	87
5			Eicosane	282	C20H42	000112-95-8	86



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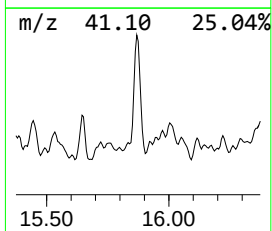
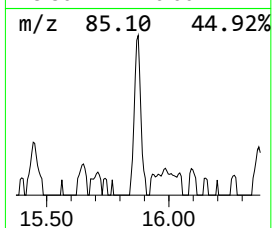
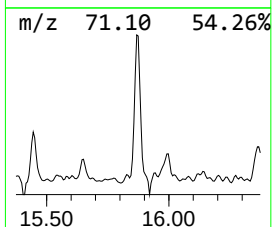
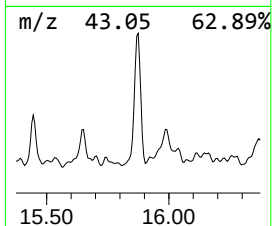
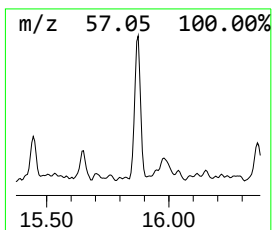
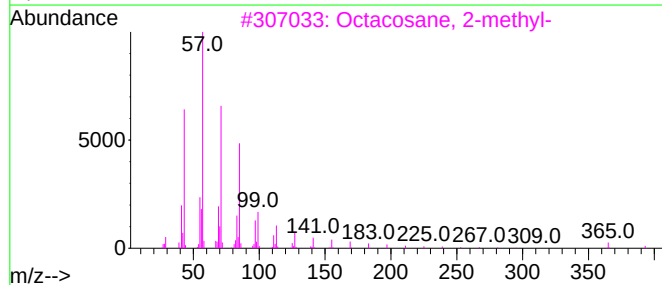
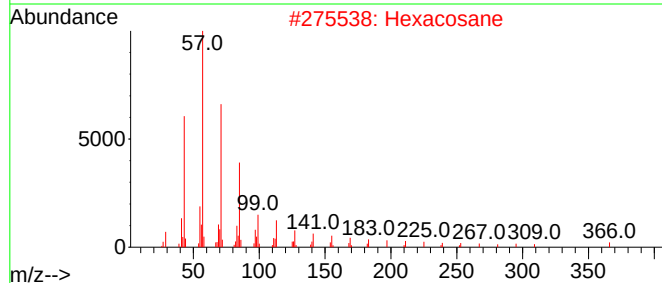
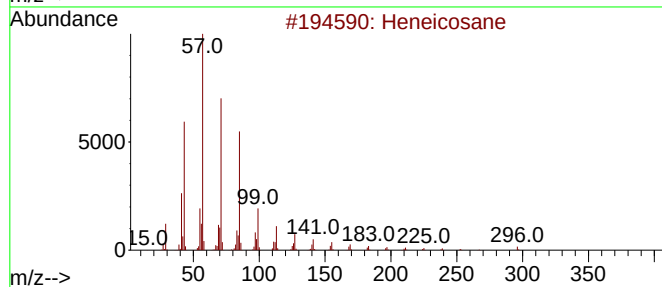
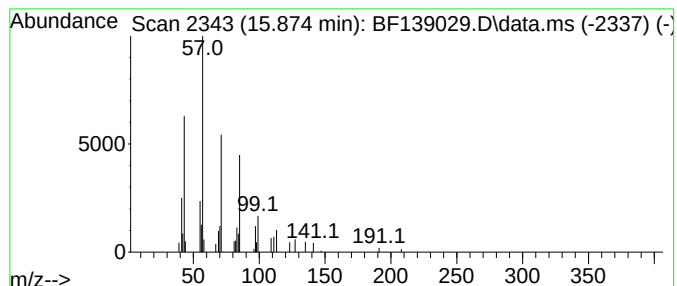
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	2.97 ng	28211	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139029.D
Acq On : 15 Aug 2024 18:40
Operator : RC/JU
Sample : P3580-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
923-K1-SD-0-0.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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
2-Pentanone, 4-...	5.057	3.8	ng	43591	1	6.834	231429	20.0
1-Phenoxypropan...	8.434	3.0	ng	45012	2	8.116	302369	20.0
Ethanol, 2-(tet...	13.827	4.0	ng	38343	5	13.998	193155	20.0
unknown13.886	13.886	5.3	ng	51575	5	13.998	193155	20.0
Heneicosane	15.074	5.7	ng	54501	6	15.463	189855	20.0
Hexacosane	15.874	3.0	ng	28211	6	15.463	189855	20.0