

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
 Data File : BM047443.D
 Acq On : 04 Sep 2024 18:02
 Operator : RC/JU
 Sample : P3750-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 346

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_M\Methods\8270-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047443.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.269	62	65	75	rBV	43271	81387	1.80%	0.221%
2	4.557	278	284	292	rBV	102079	149600	3.31%	0.407%
3	5.010	355	361	382	rBV	1575900	2442150	54.07%	6.640%
4	6.575	621	627	642	rBV	1284522	2369659	52.47%	6.443%
5	6.986	692	697	705	rBV2	30517	72891	1.61%	0.198%
6	7.339	750	757	767	rBV	862877	1369754	30.33%	3.724%
7	8.492	946	953	968	rBV	815816	1563225	34.61%	4.250%
8	10.098	1218	1226	1244	rBV	915044	1666645	36.90%	4.532%
9	10.874	1351	1358	1373	rBV2	70878	199699	4.42%	0.543%
10	12.610	1645	1653	1672	rBV	2104419	3502074	77.54%	9.522%
11	14.004	1884	1890	1898	rBV	1327253	2077705	46.01%	5.649%
12	14.068	1899	1901	1910	rVB	45263	76902	1.70%	0.209%
13	14.239	1925	1930	1931	rBV	77119	103694	2.30%	0.282%
14	14.257	1931	1933	1940	rVB2	85956	111015	2.46%	0.302%
15	15.080	2065	2073	2077	rBV4	24003	45665	1.01%	0.124%
16	15.527	2143	2149	2159	rBV	1594423	2558366	56.65%	6.956%
17	15.774	2186	2191	2198	rVB7	21924	48640	1.08%	0.132%
18	16.774	2355	2361	2366	rBV	1562454	2335492	51.71%	6.350%
19	16.815	2366	2368	2377	rVV	252480	413432	9.15%	1.124%
20	16.915	2380	2385	2391	rVB	72258	125394	2.78%	0.341%
21	17.474	2477	2480	2483	rBV3	36575	46089	1.02%	0.125%
22	17.656	2506	2511	2515	rBV	90051	135115	2.99%	0.367%
23	17.709	2515	2520	2528	rBV	533760	840797	18.62%	2.286%
24	17.845	2539	2543	2547	rBV3	109808	185726	4.11%	0.505%
25	17.886	2548	2550	2557	rVB	67321	94846	2.10%	0.258%
26	18.168	2594	2598	2603	rBV	41885	58644	1.30%	0.159%
27	18.592	2666	2670	2674	rBV	75962	116605	2.58%	0.317%
28	18.856	2710	2715	2723	rBV	661747	924871	20.48%	2.515%
29	19.009	2737	2741	2750	rBV2	263335	430142	9.52%	1.170%
30	19.221	2769	2777	2788	rBV	639015	1071589	23.73%	2.914%
31	19.439	2809	2814	2828	rVB	3655076	4516257	100.00%	12.280%
32	20.033	2912	2915	2919	rBV	75476	90171	2.00%	0.245%
33	20.739	3032	3035	3042	rVB4	399468	540597	11.97%	1.470%
34	21.021	3077	3083	3087	rBV2	2062275	3138811	69.50%	8.534%
35	21.062	3087	3090	3095	rVB	386028	527163	11.67%	1.433%
36	23.727	3536	3543	3551	rBV	1248097	2747927	60.85%	7.472%

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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_M\Methods\8270-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

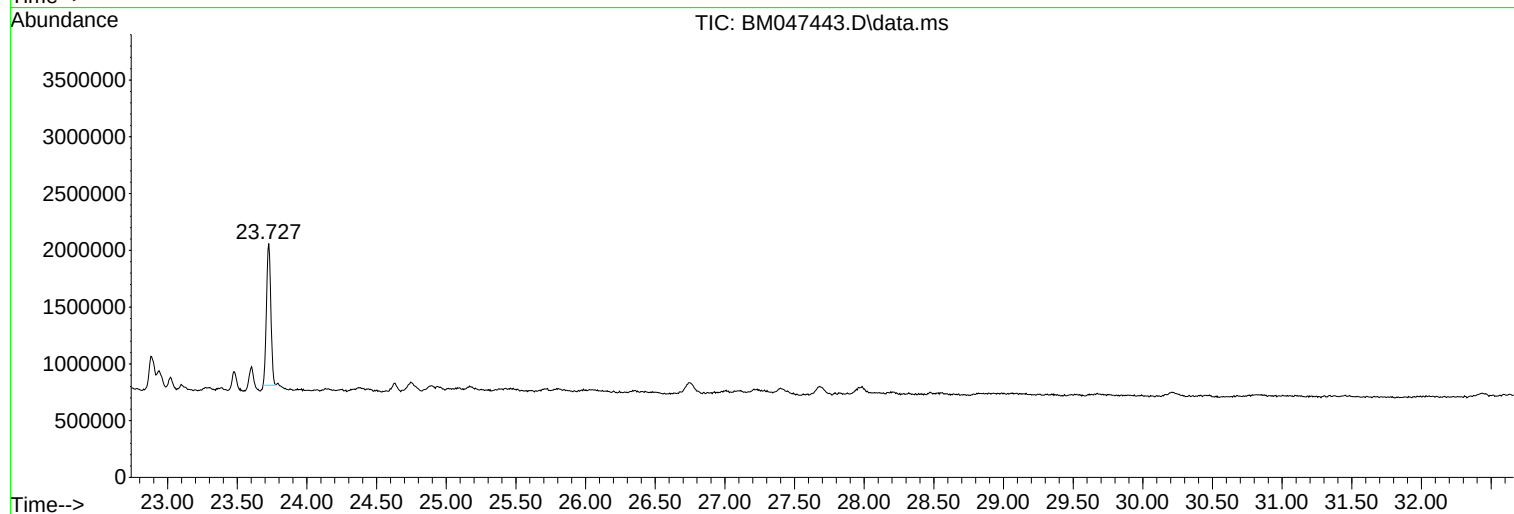
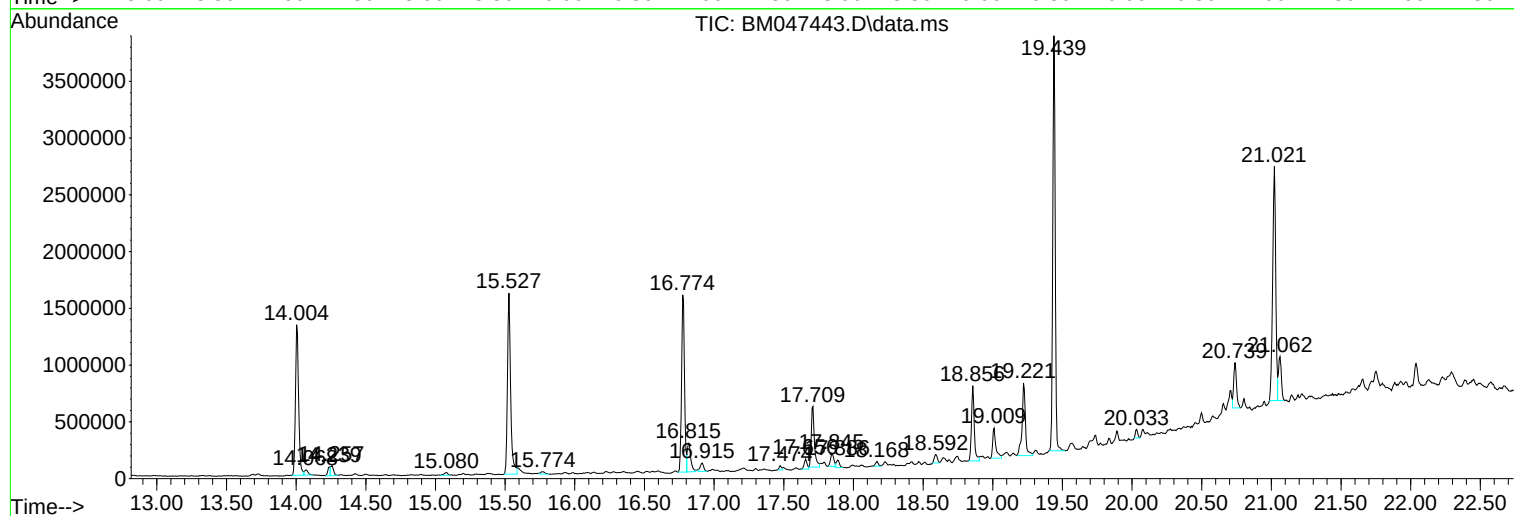
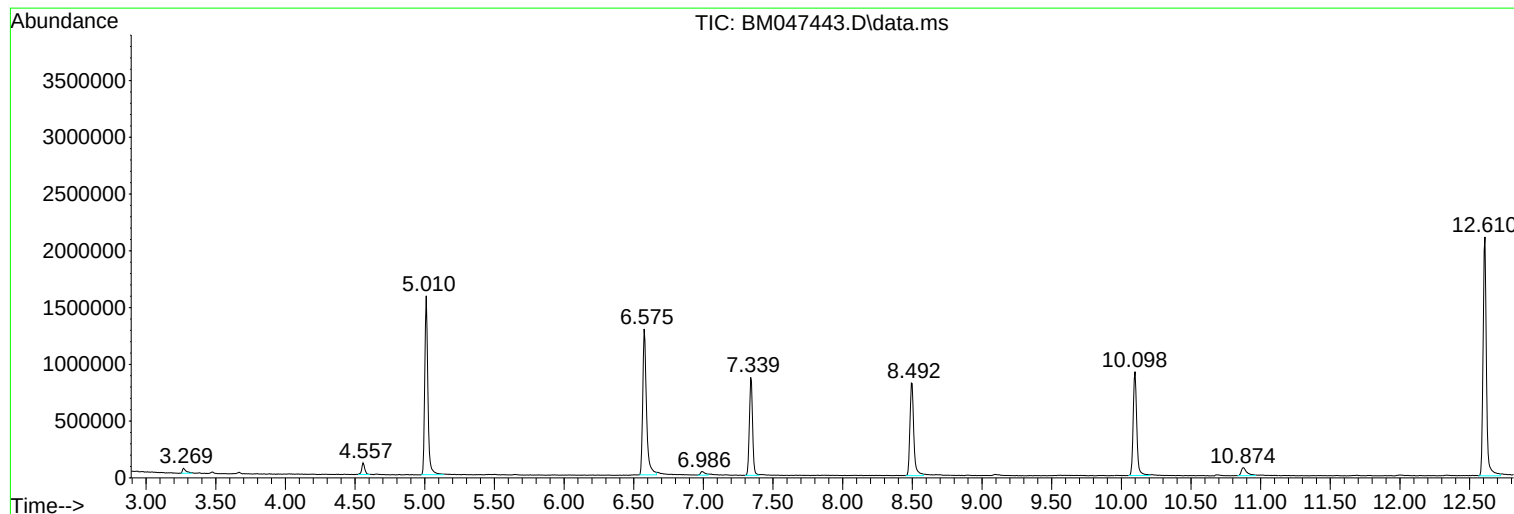
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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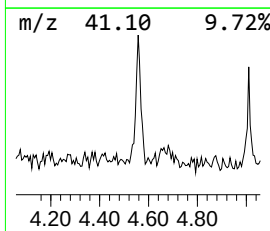
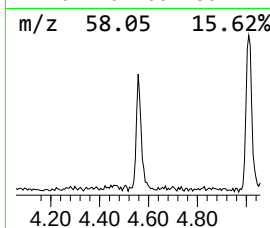
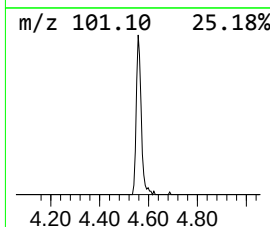
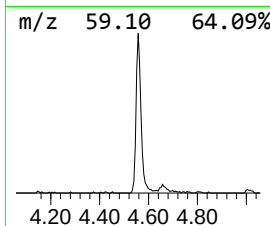
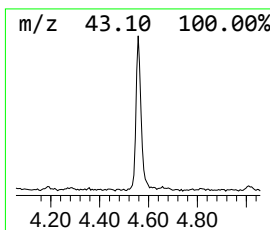
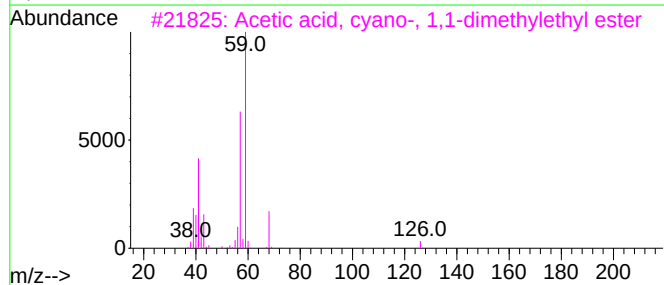
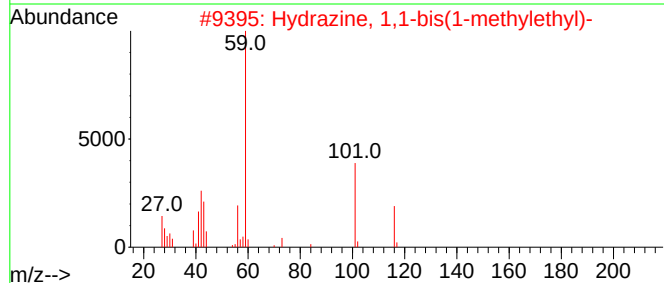
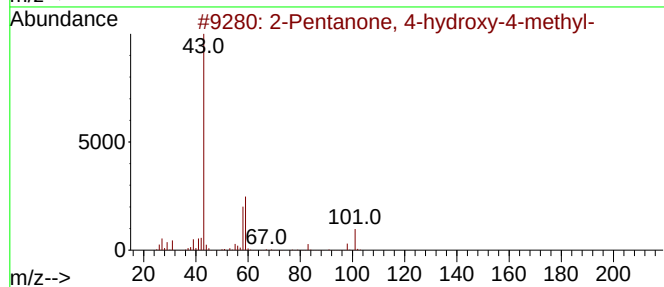
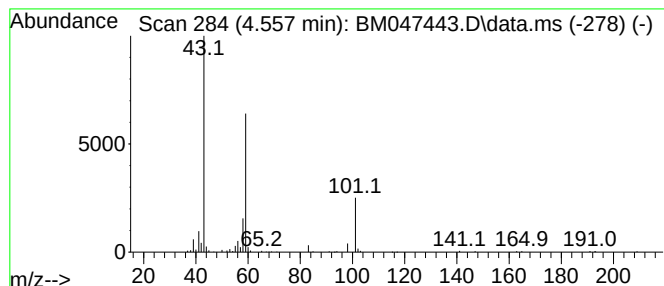
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	2.18 ng	149600	1,4-Dichlorobenzene-d4	7.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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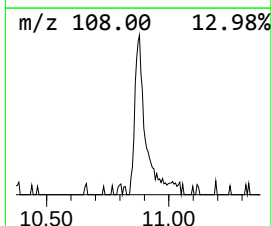
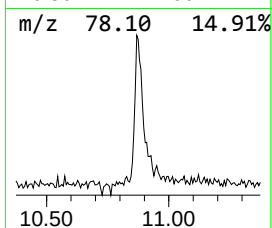
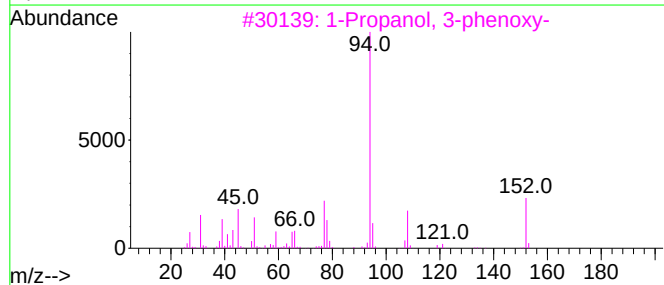
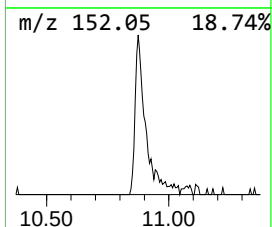
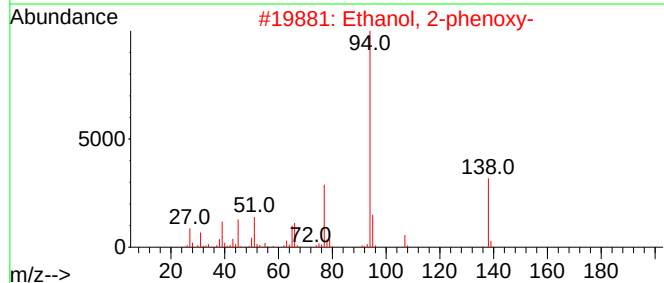
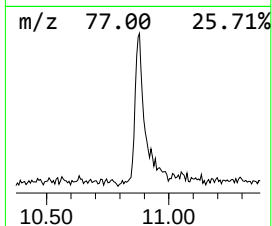
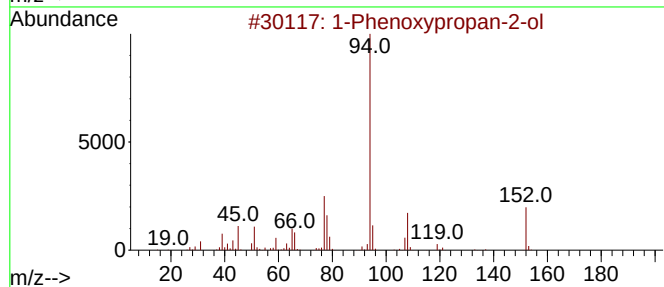
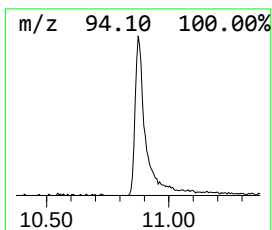
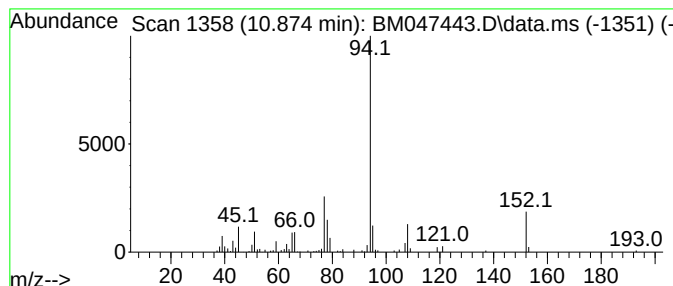
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.874	2.40 ng	199699	Naphthalene-d8	10.098

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
3		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
4		Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	59
5		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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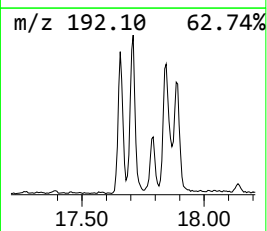
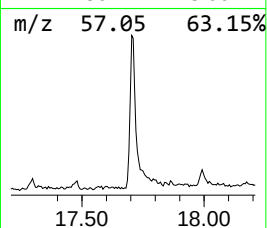
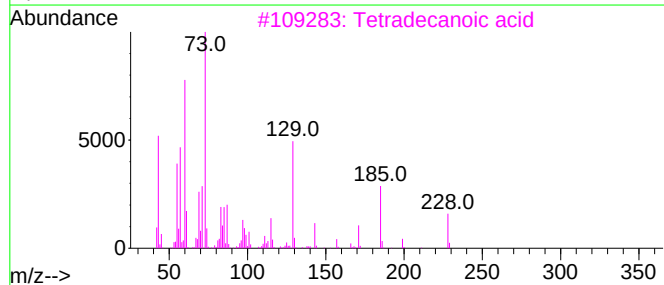
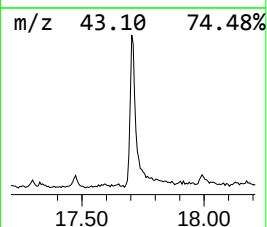
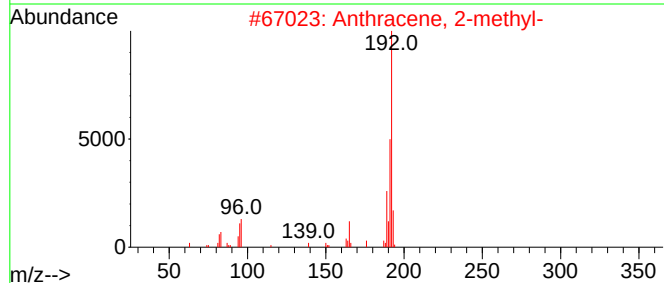
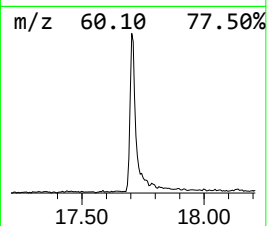
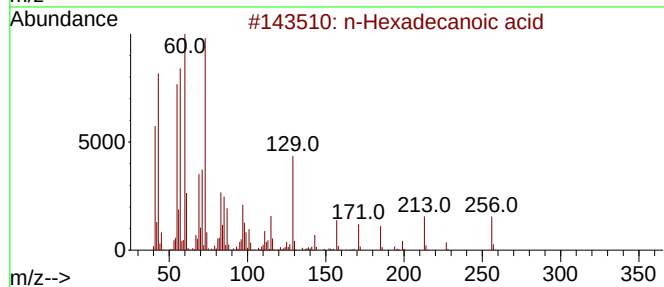
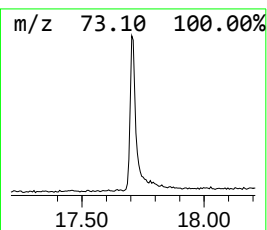
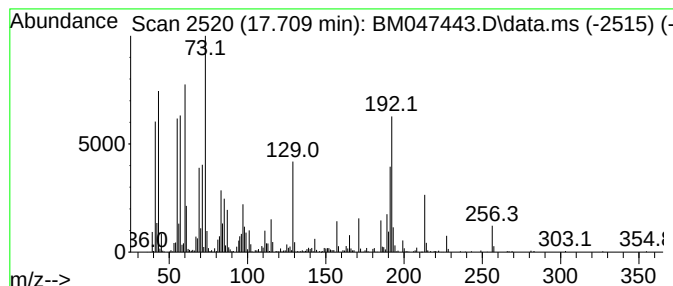
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	7.20 ng	840797	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	78
4			Octadecanoic acid	284	C18H36O2	000057-11-4	70
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	70



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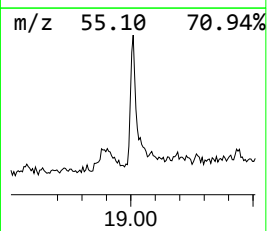
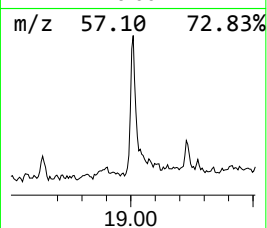
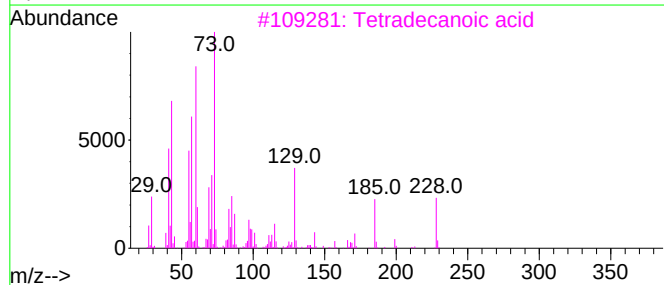
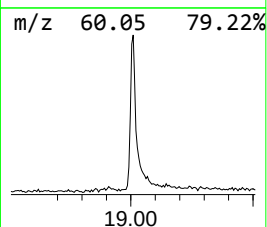
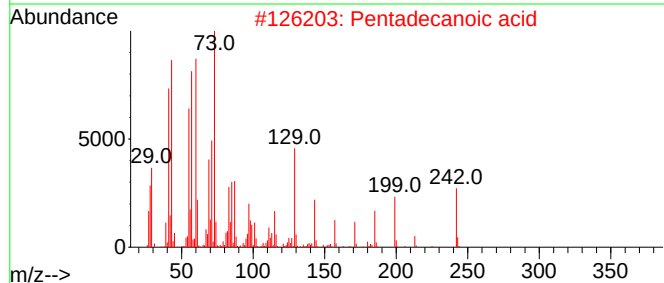
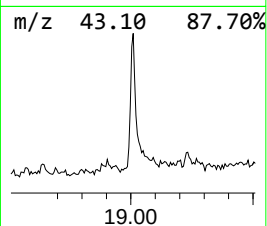
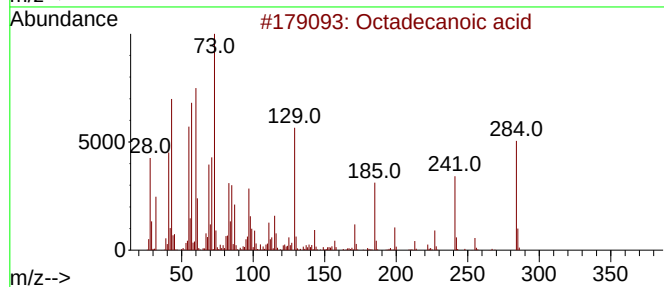
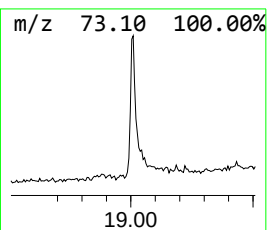
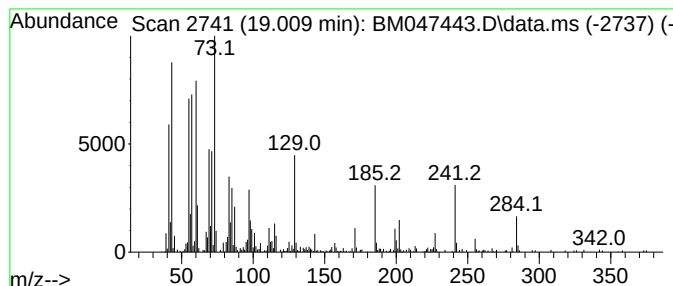
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	2.74 ng	430142	Chrysene-d12	21.021

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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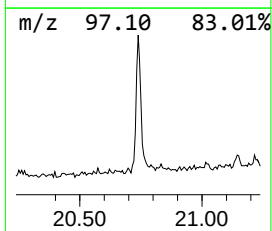
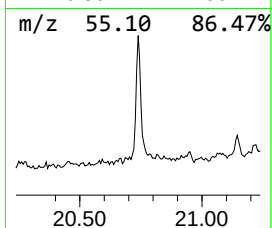
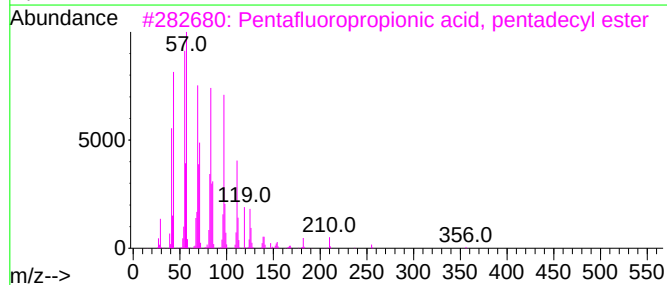
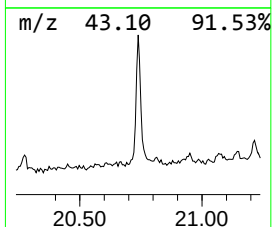
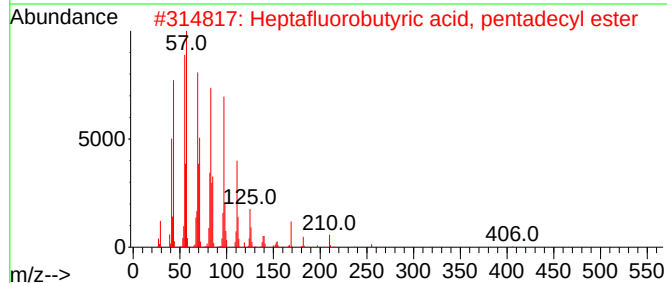
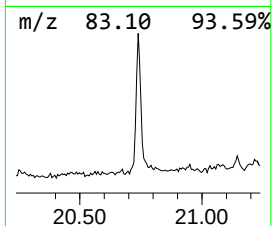
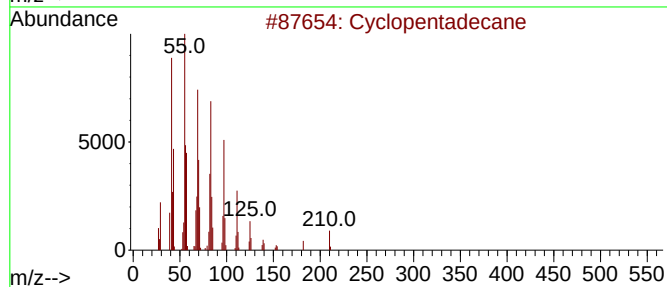
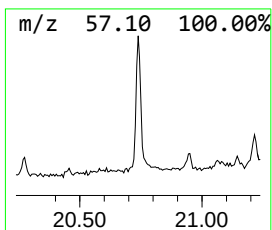
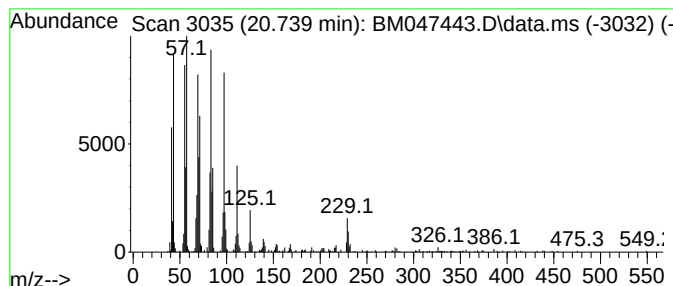
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.738	3.44 ng	540597	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	93
5			1-Heptacosanol	396	C27H56O	002004-39-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
Data File : BM047443.D
Acq On : 04 Sep 2024 18:02
Operator : RC/JU
Sample : P3750-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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-...	4.557	2.2	ng	149600	1	7.339	1369750	20.0
1-Phenoxypropan...	10.874	2.4	ng	199699	2	10.098	1666650	20.0
n-Hexadecanoic ...	17.709	7.2	ng	840797	4	16.774	2335490	20.0
Octadecanoic acid	19.009	2.7	ng	430142	5	21.021	3138810	20.0
Cyclopentadecane	20.738	3.4	ng	540597	5	21.021	3138810	20.0