

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
 Data File : BM047235.D
 Acq On : 16 Aug 2024 15:11
 Operator : RC/JU
 Sample : P3582-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S-855-J-SO-1.5-2-081224-FD

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047235.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.263	61	64	72	rBV	98937	130540	2.17%	0.301%
2	4.575	281	287	297	rVB	171706	246119	4.10%	0.567%
3	5.016	356	362	380	rVB	2684862	3774589	62.88%	8.699%
4	6.575	620	627	643	rBV	2481294	3797910	63.27%	8.753%
5	7.363	754	761	770	rBV	984037	1473999	24.56%	3.397%
6	8.510	949	956	966	rBV	1552997	2505577	41.74%	5.775%
7	9.092	1050	1055	1061	rBV	42129	68255	1.14%	0.157%
8	10.116	1218	1229	1239	rBV	1138866	1828208	30.46%	4.213%
9	10.881	1351	1359	1370	rBV	136740	289588	4.82%	0.667%
10	12.628	1648	1656	1666	rBV	3443007	5036961	83.91%	11.609%
11	14.022	1886	1893	1901	rBV	1478840	2155846	35.91%	4.969%
12	14.257	1927	1933	1934	rBV	72973	85463	1.42%	0.197%
13	14.274	1934	1936	1943	rVB2	84219	111728	1.86%	0.257%
14	15.527	2143	2149	2163	rBV	2452665	3622495	60.35%	8.349%
15	16.786	2357	2363	2367	rBV	1604916	2310309	38.49%	5.325%
16	16.827	2367	2370	2376	rVB	157492	210298	3.50%	0.485%
17	16.915	2381	2385	2393	rVB	70805	106944	1.78%	0.246%
18	17.721	2517	2522	2540	rBV	596596	1096771	18.27%	2.528%
19	18.262	2609	2614	2621	rBV	61986	110989	1.85%	0.256%
20	18.862	2711	2716	2720	rBV	299475	425905	7.10%	0.982%
21	19.021	2739	2743	2751	rBV	242234	397804	6.63%	0.917%
22	19.174	2765	2769	2772	rBV	146815	177506	2.96%	0.409%
23	19.227	2772	2778	2782	rVB	229553	346743	5.78%	0.799%
24	19.451	2811	2816	2827	rVB	5011286	6002812	100.00%	13.835%
25	20.233	2946	2949	2950	rBV2	111873	109045	1.82%	0.251%
26	20.768	3036	3040	3048	rBV3	228366	404002	6.73%	0.931%
27	21.021	3077	3083	3088	rBV	1972825	2826733	47.09%	6.515%
28	22.733	3370	3374	3382	rVB	436824	754935	12.58%	1.740%
29	23.715	3534	3541	3557	rVB	1235751	2982056	49.68%	6.873%

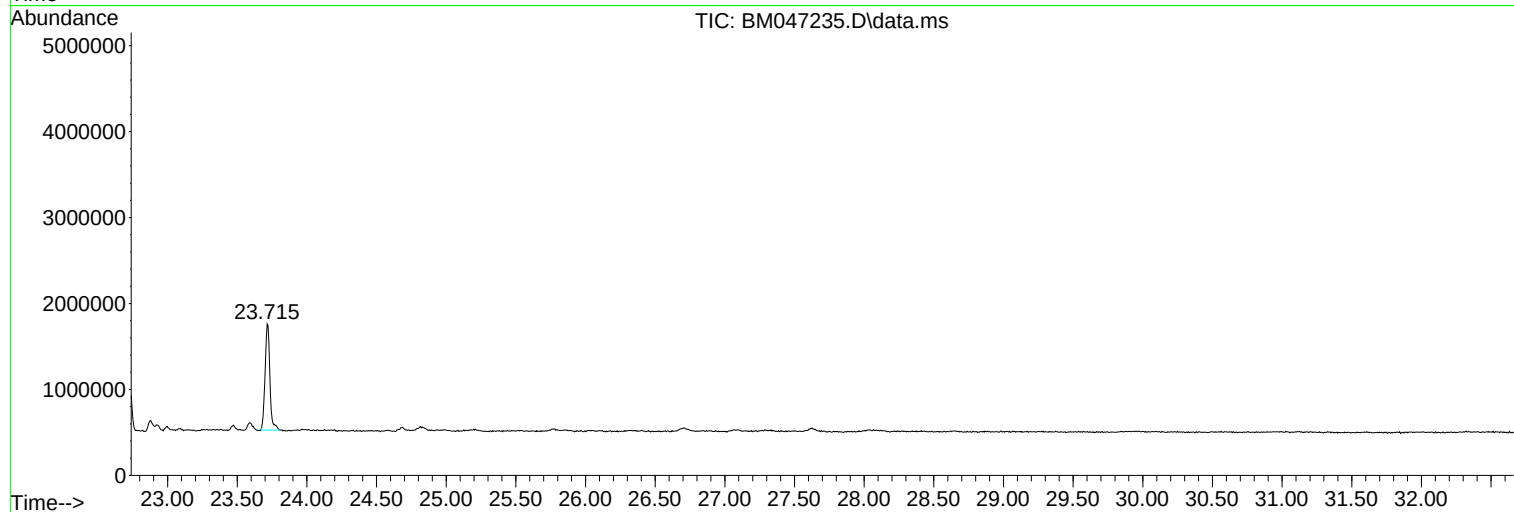
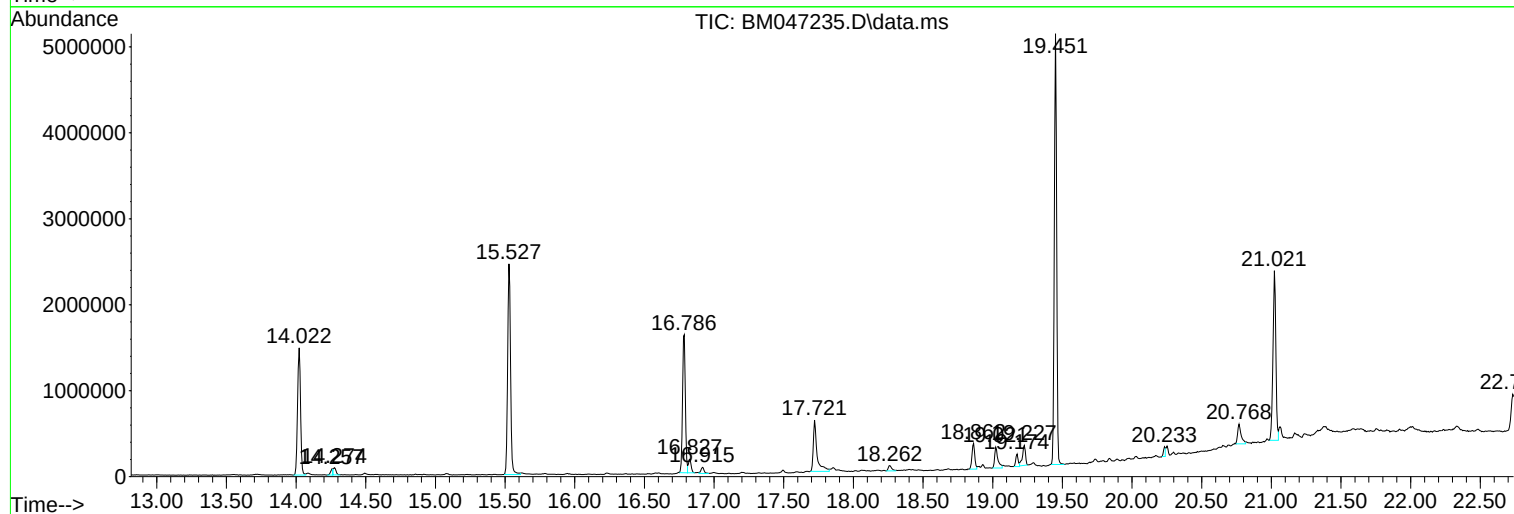
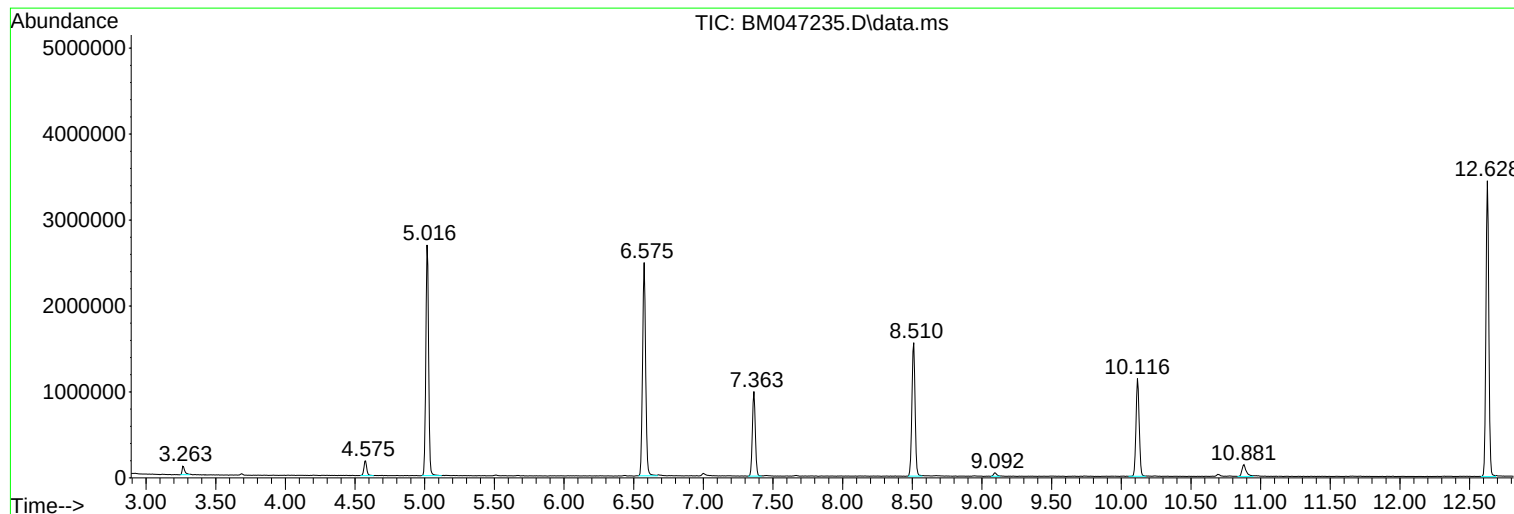
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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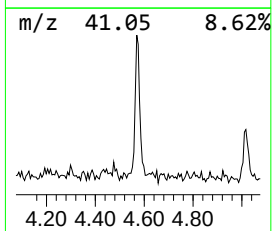
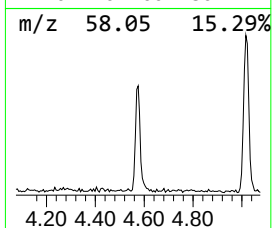
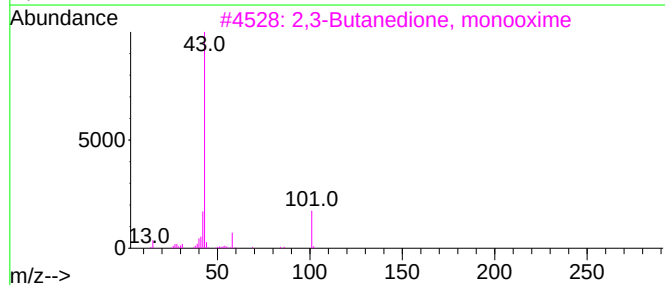
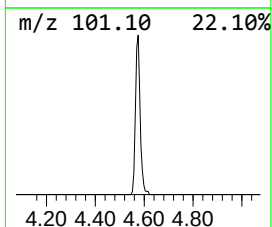
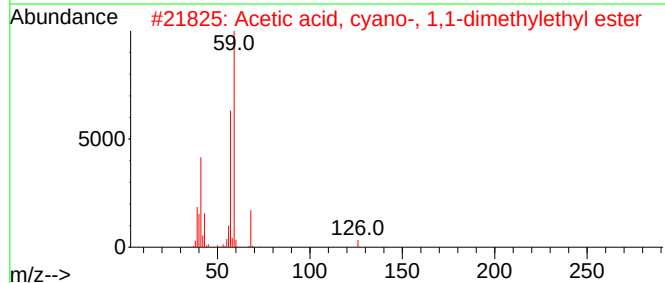
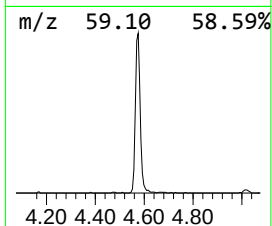
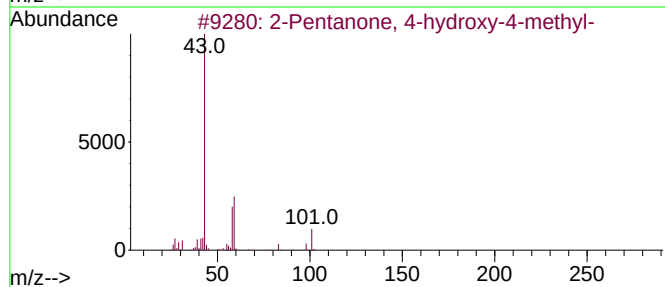
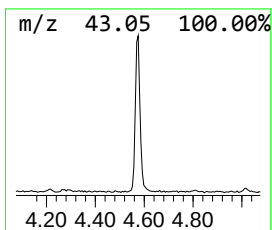
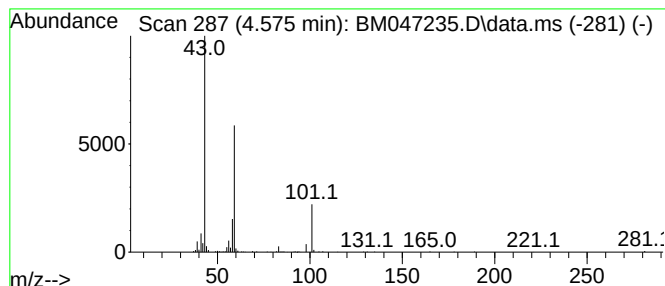
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.575	3.34 ng	246119	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	Hexanamide	115	C6H13NO	000628-02-4	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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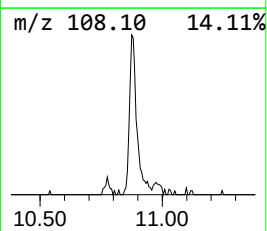
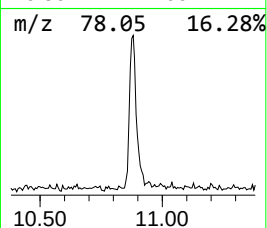
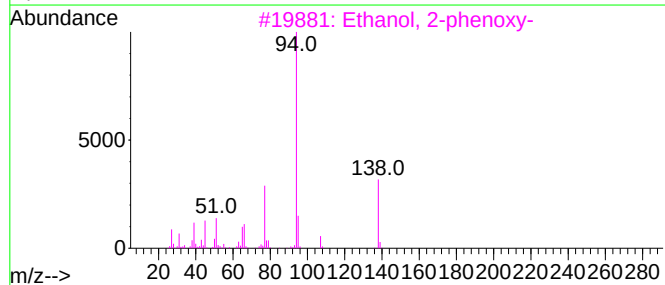
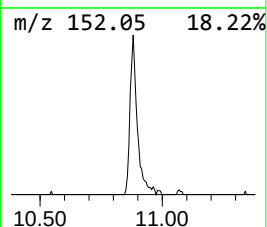
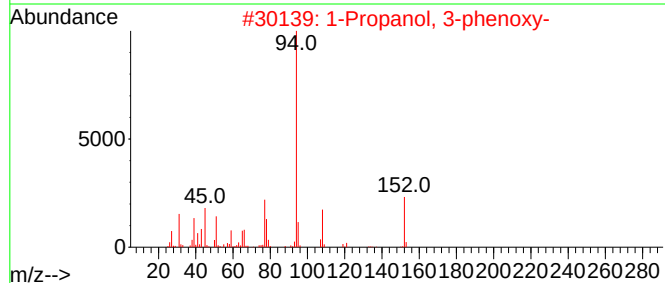
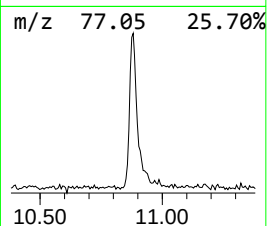
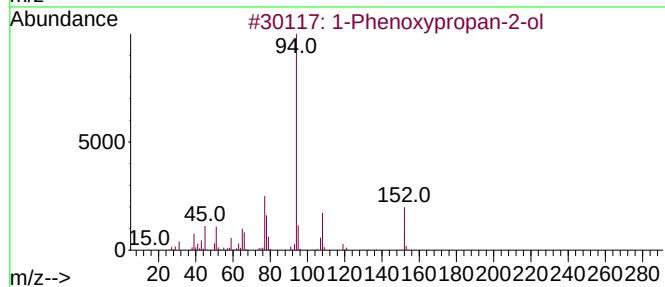
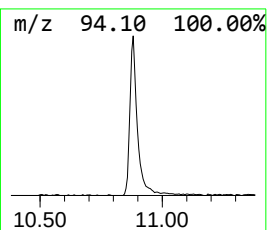
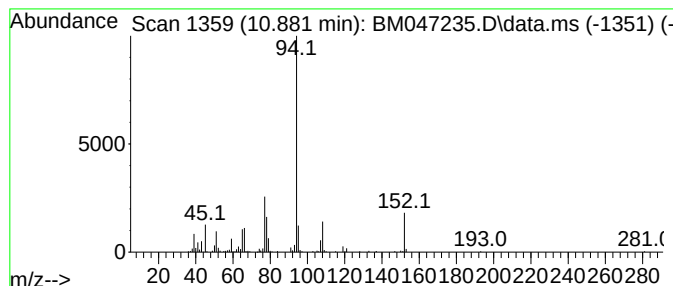
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	3.17 ng	289588	Naphthalene-d8	10.116

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	83
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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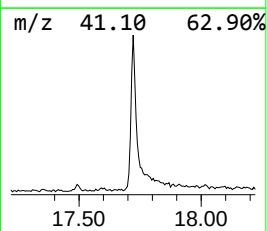
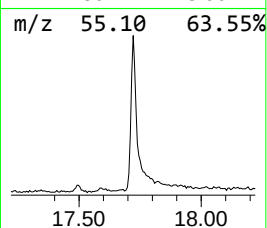
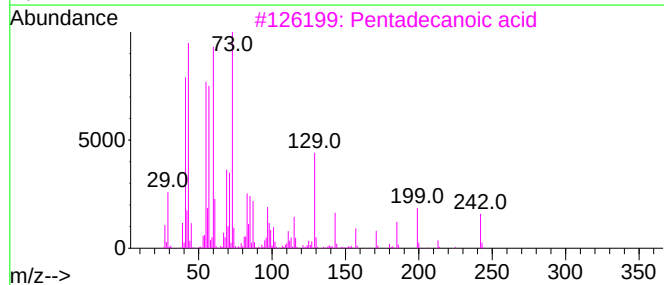
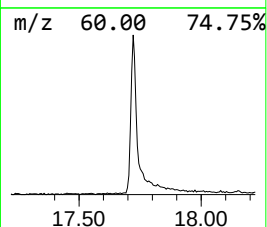
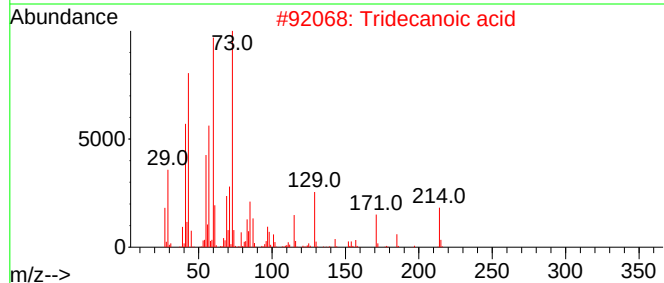
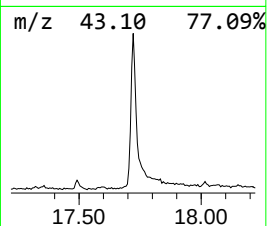
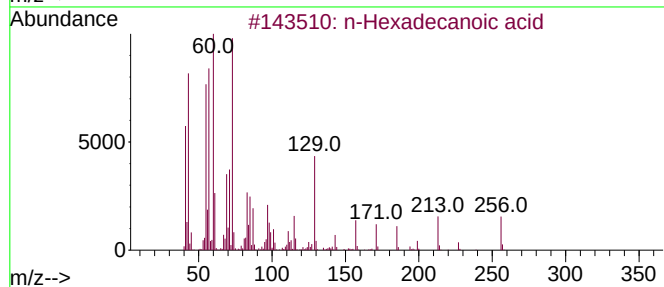
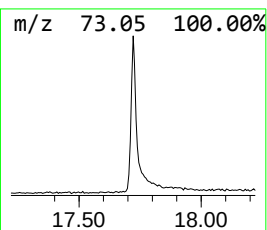
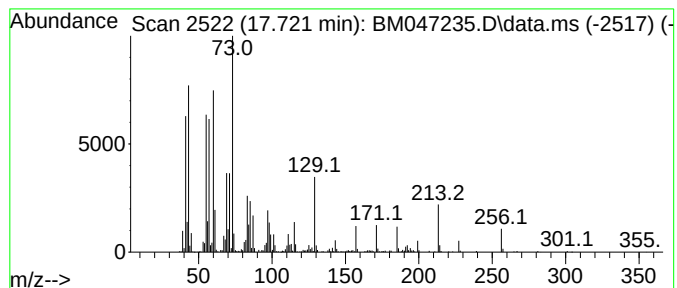
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	9.49 ng	1096770	Phenanthrene-d10	16.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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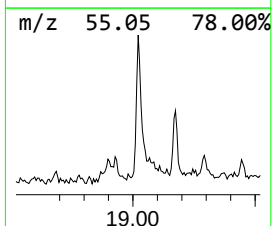
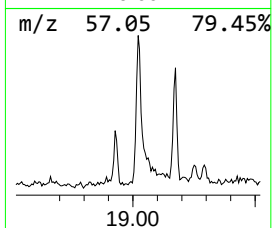
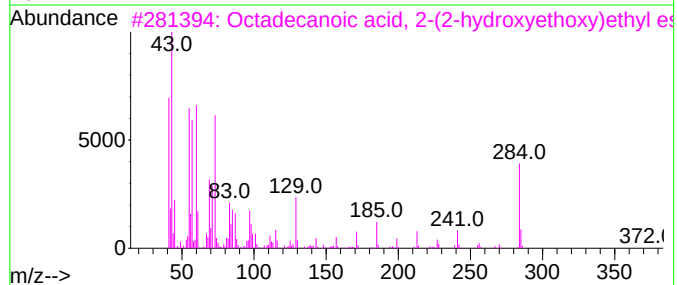
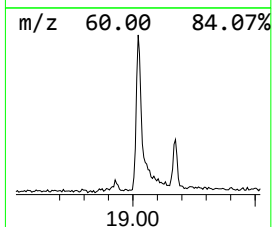
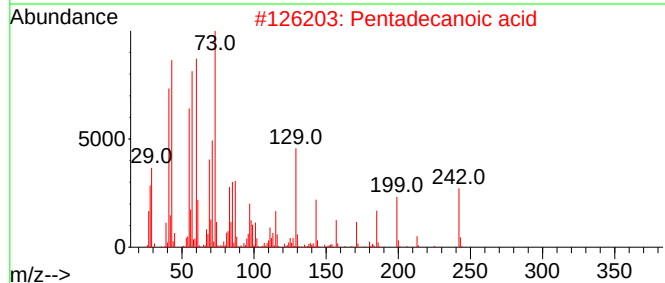
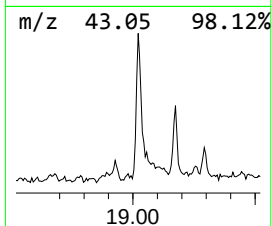
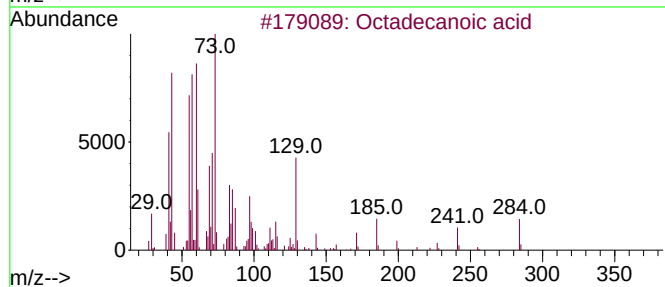
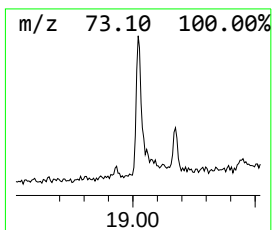
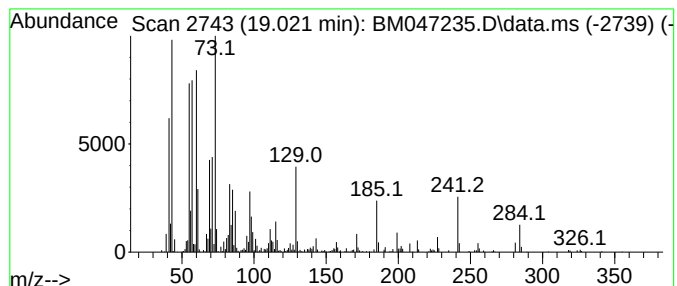
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.021	2.81 ng	397804	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	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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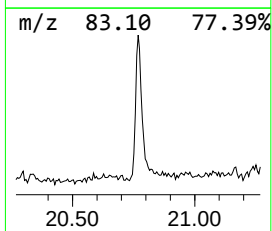
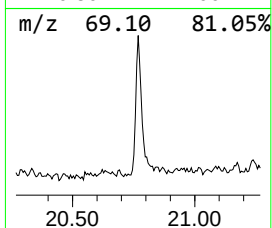
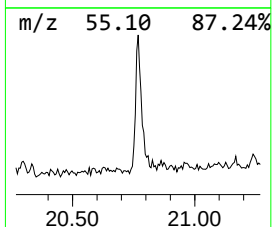
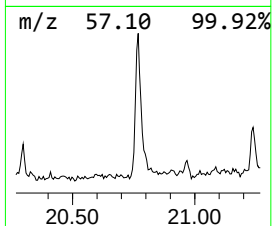
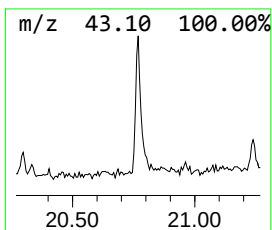
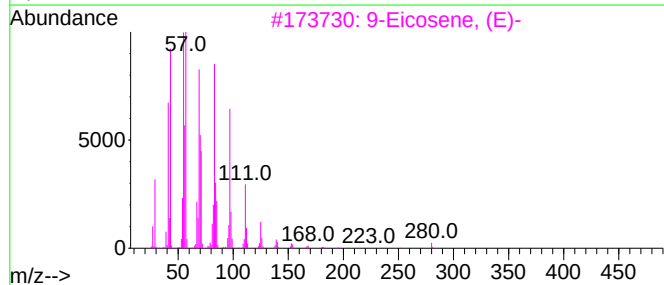
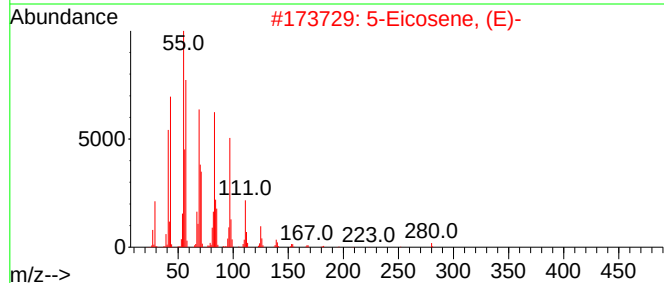
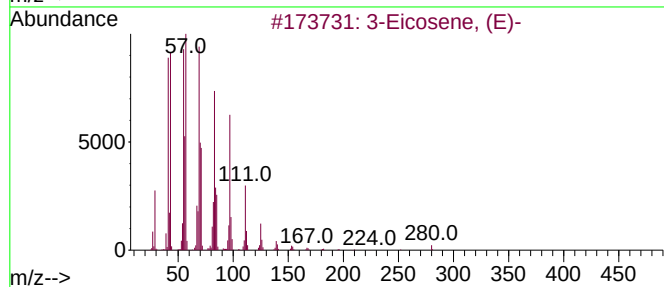
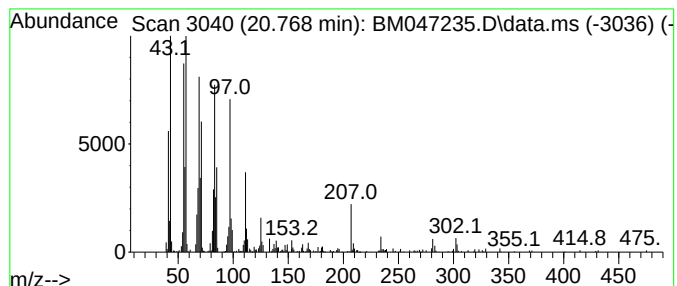
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Peak Number 5 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.768	2.86 ng	404002	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	97
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5			1-Eicosene	280	C20H40	003452-07-1	91



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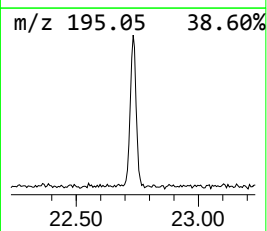
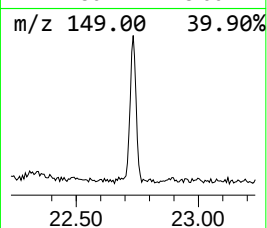
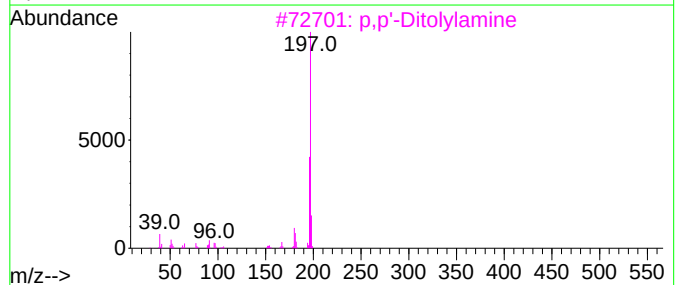
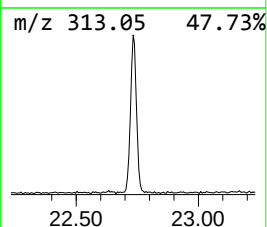
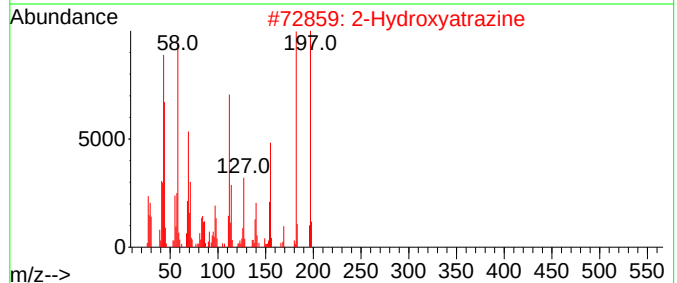
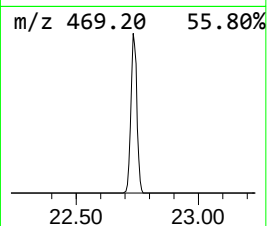
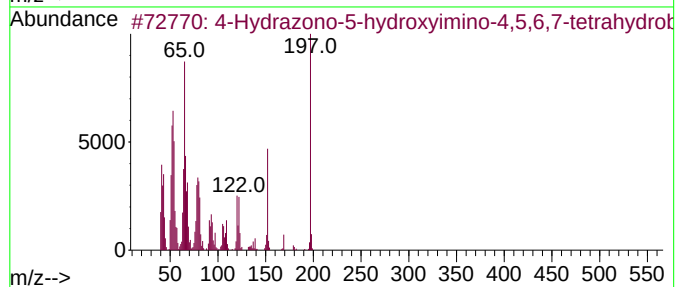
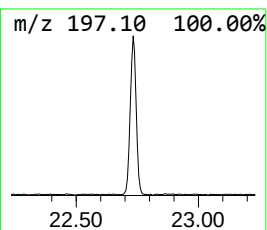
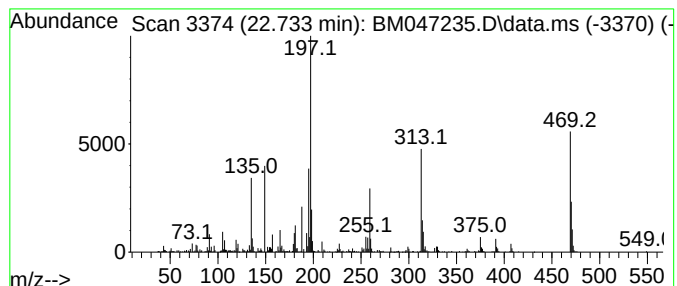
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown22.733 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.733	5.06 ng	754935	Perylene-d12	23.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Hydrazono-5-hydroxyimino-4,5,6...	197	C6H7N5O3	303194-86-7	25
2			2-Hydroxyatrazine	197	C8H15N5O	002163-68-0	25
3			p,p'-Ditolylamine	197	C14H15N	000620-93-9	18
4			Glutaric acid, monoamide, N,N-di...	353	C22H27N03	1000360-23-0	14
5			Pyridinium, 1-[(hydroxyphenylmet...	212	C13H12N2O	017408-47-8	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047235.D
Acq On : 16 Aug 2024 15:11
Operator : RC/JU
Sample : P3582-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-1.5-2-081224-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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-...	4.575	3.3	ng	246119	1	7.363	1474000	20.0
1-Phenoxypropan...	10.881	3.2	ng	289588	2	10.116	1828210	20.0
n-Hexadecanoic ...	17.721	9.5	ng	1096770	4	16.786	2310310	20.0
Octadecanoic acid	19.021	2.8	ng	397804	5	21.021	2826730	20.0
3-Eicosene, (E)-	20.768	2.9	ng	404002	5	21.021	2826730	20.0
unknown22.733	22.733	5.1	ng	754935	6	23.715	2982060	20.0