

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
 Data File : BM039392.D
 Acq On : 11 Apr 2023 13:46
 Operator : CG/JU
 Sample : 02256-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 360

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-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.951	293	300	310	rBV	874123	1255214	35.97%	3.262%
2	5.422	374	380	398	rBV	1918730	2937950	84.19%	7.635%
3	7.034	647	654	668	rBV	1804331	3028382	86.78%	7.870%
4	7.863	788	795	807	rBV	585322	971630	27.84%	2.525%
5	9.034	986	994	1014	rBV	980398	1790981	51.32%	4.654%
6	10.675	1264	1273	1285	rBV	733228	1344246	38.52%	3.493%
7	13.139	1685	1692	1707	rBV	1423744	2237928	64.13%	5.816%
8	13.457	1739	1746	1763	rBV	55444	201912	5.79%	0.525%
9	14.516	1919	1926	1942	rBV	1156937	1786085	51.18%	4.642%
10	14.939	1993	1998	2006	rBV2	23774	53141	1.52%	0.138%
11	15.880	2151	2158	2169	rBV	285444	448876	12.86%	1.167%
12	16.010	2173	2180	2200	rVV	2310288	3361276	96.32%	8.735%
13	16.674	2288	2293	2299	rBV7	23125	49524	1.42%	0.129%
14	17.268	2388	2394	2398	rBV	1418677	2054480	58.87%	5.339%
15	17.309	2398	2401	2410	rVV	258621	382723	10.97%	0.995%
16	17.398	2411	2416	2421	rVV	64243	106183	3.04%	0.276%
17	18.168	2539	2547	2562	rBV	1250136	2243002	64.28%	5.829%
18	18.345	2572	2577	2581	rBV3	61342	106853	3.06%	0.278%
19	18.651	2625	2629	2633	rBV	31360	45554	1.31%	0.118%
20	18.698	2635	2637	2643	rVB5	28433	40067	1.15%	0.104%
21	19.327	2737	2744	2752	rBV	1109235	1661763	47.62%	4.319%
22	19.445	2760	2764	2777	rBV	596221	1067926	30.60%	2.775%
23	19.692	2802	2806	2815	rVB	907585	1297456	37.18%	3.372%
24	19.898	2836	2841	2852	rVB	2822536	3489566	100.00%	9.069%
25	21.168	3053	3057	3065	rVB3	511519	773525	22.17%	2.010%
26	21.462	3100	3107	3111	rBV2	1932116	3306786	94.76%	8.594%
27	23.850	3507	3513	3519	rBV2	1215272	2436029	69.81%	6.331%

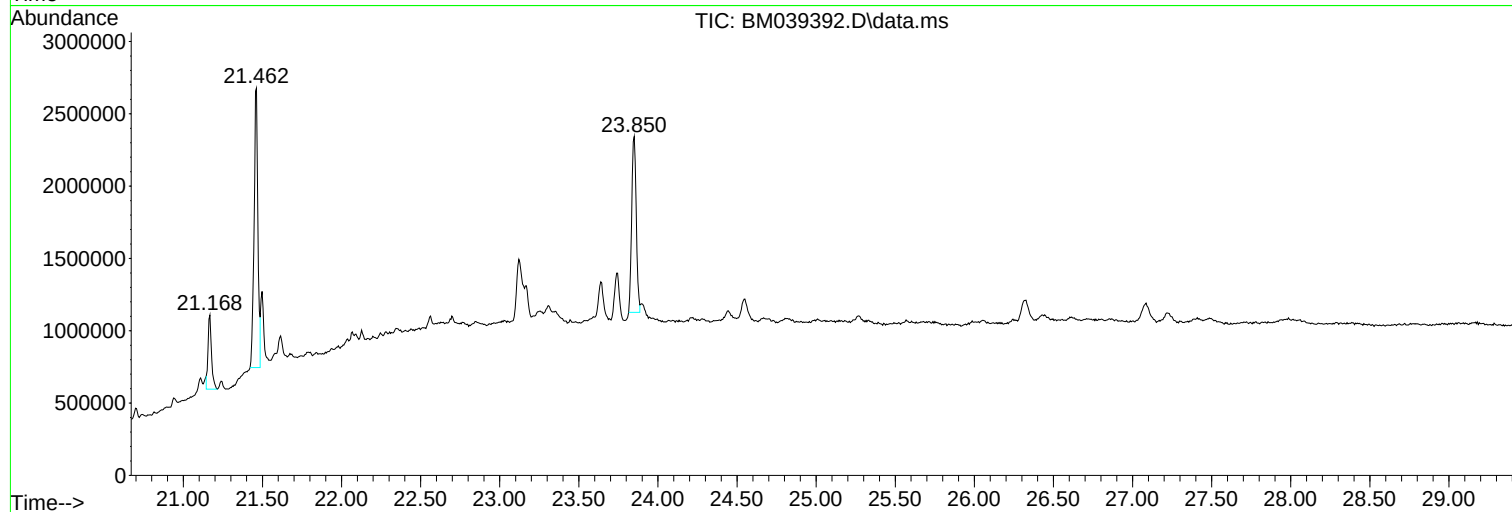
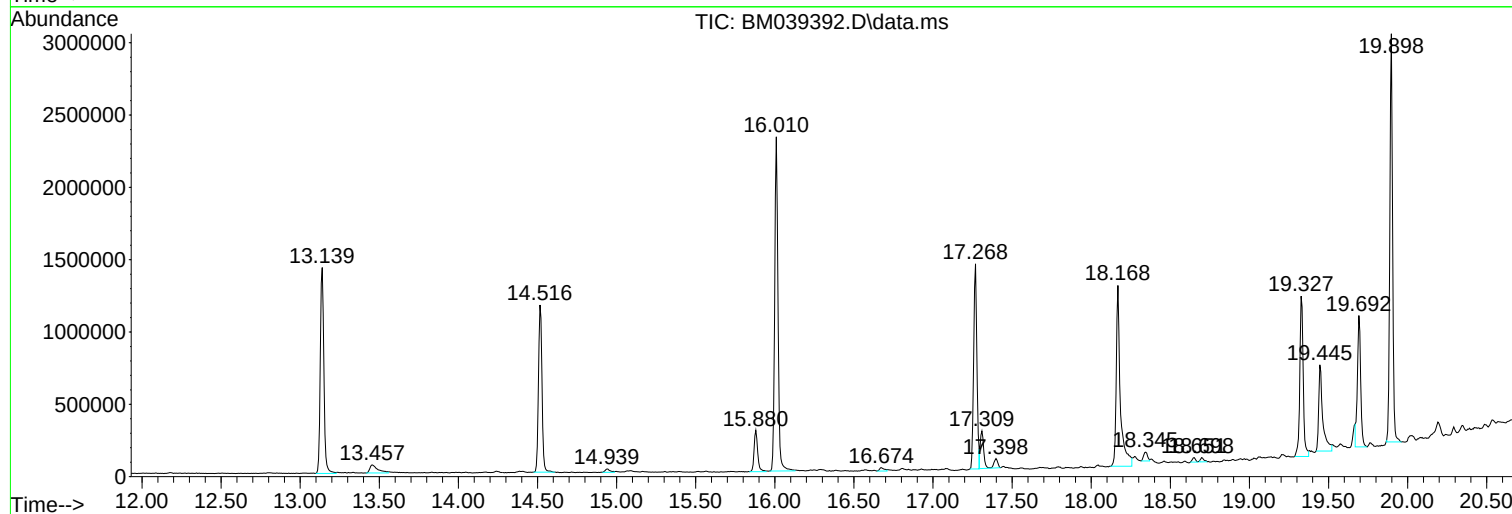
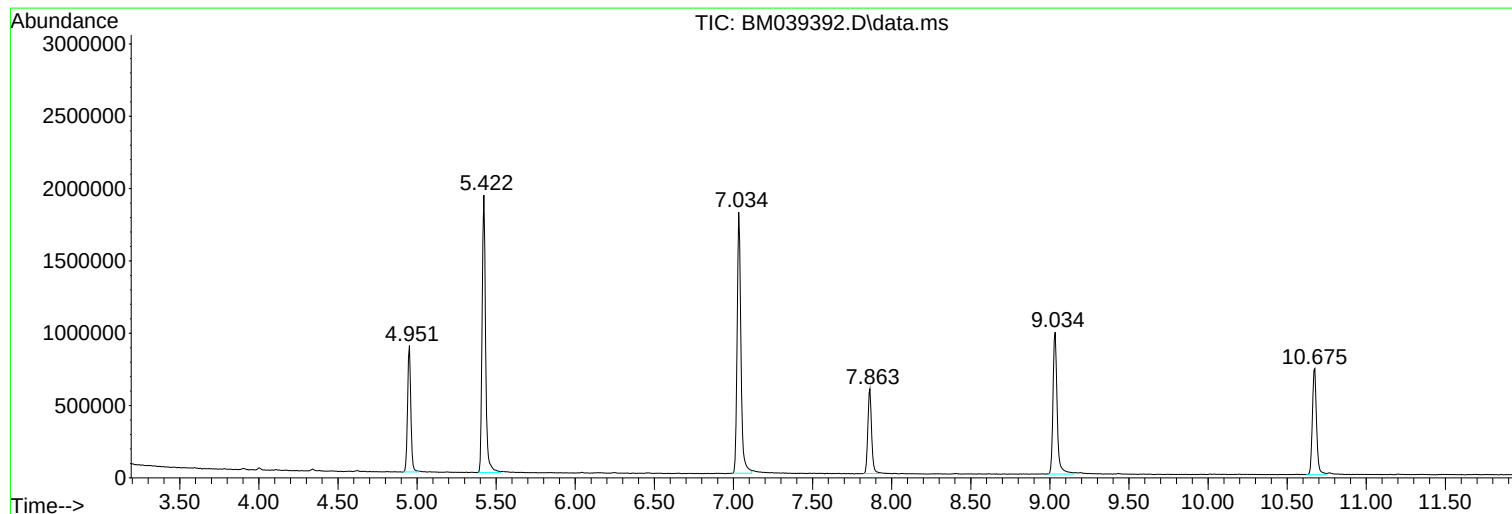
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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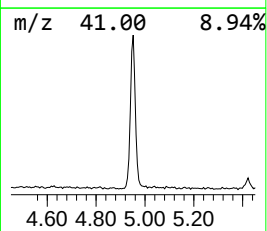
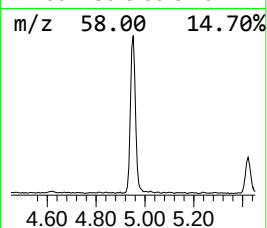
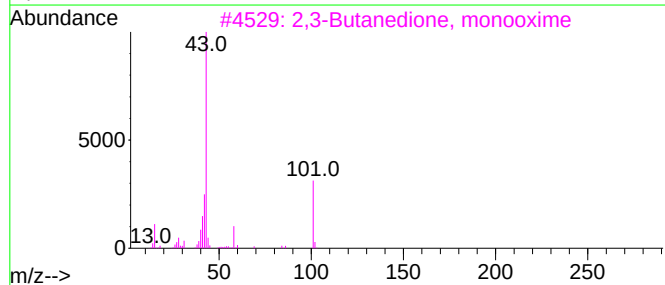
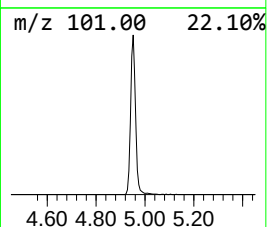
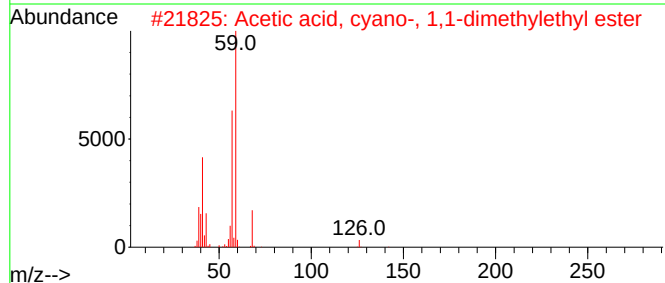
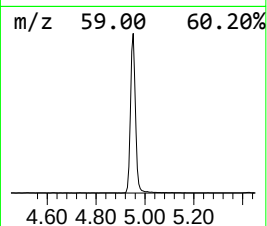
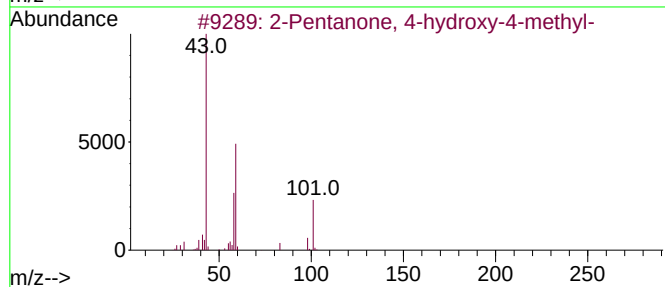
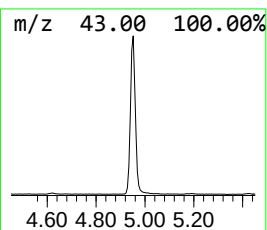
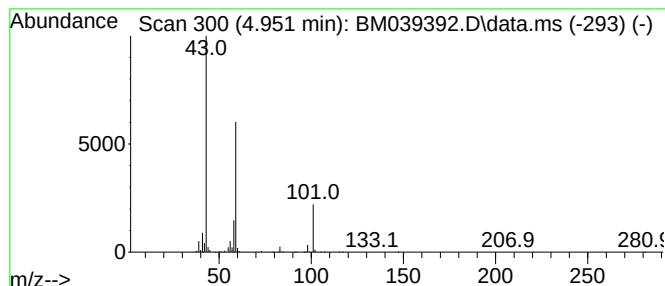
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
4.951	25.84 ng	1255210	1,4-Dichlorobenzene-d4	7.863	
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	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9



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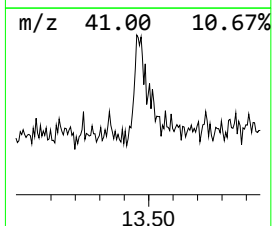
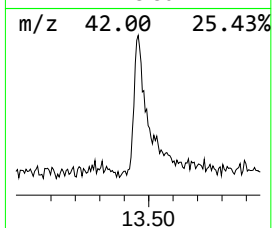
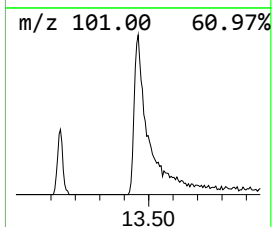
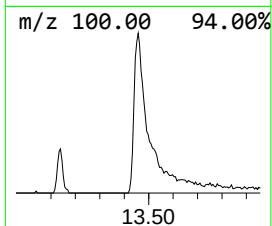
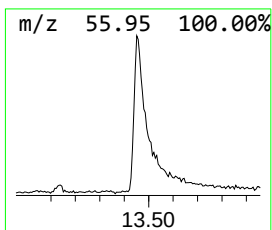
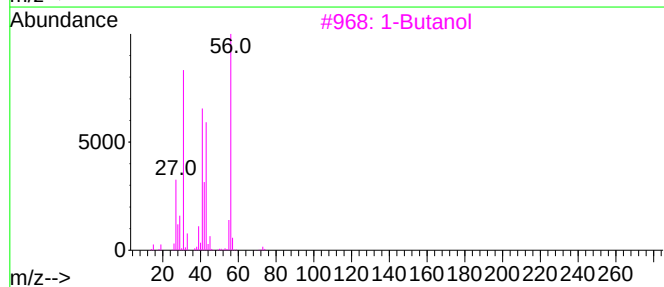
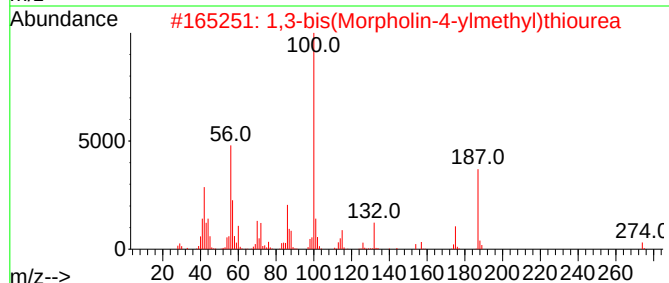
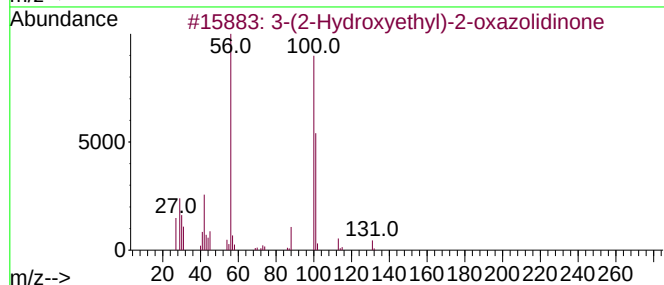
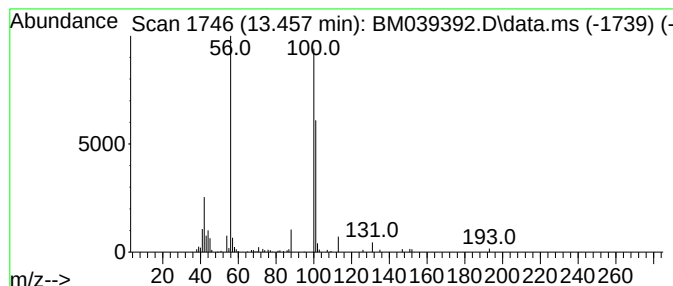
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Peak Number 2 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	2.26 ng	201912	Acenaphthene-d10	14.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	91
2			1,3-bis(Morpholin-4-ylmethyl)thi...	274	C11H22N4O2S	031411-59-3	28
3			1-Butanol	74	C4H10O	000071-36-3	27
4			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	25
5			2,2,3,3,4,4,4-Heptafluoro-N-(2-m...	326	C10H13F7N2O2	1000278-15-3	25



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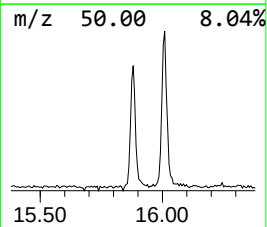
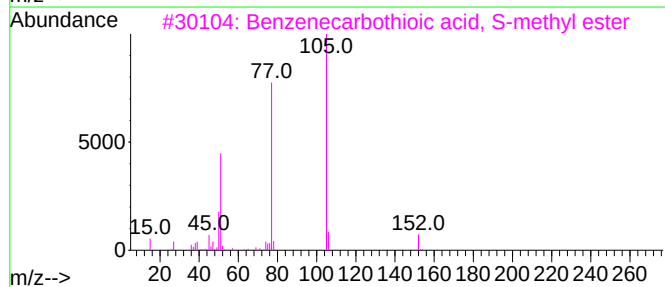
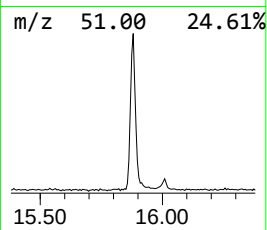
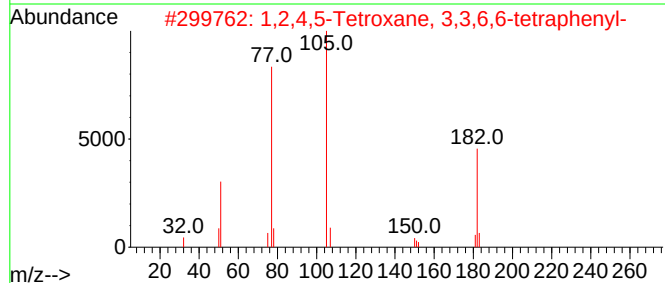
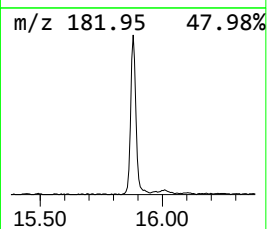
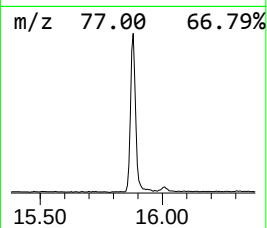
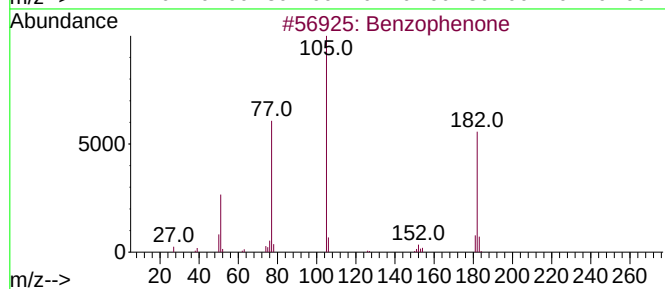
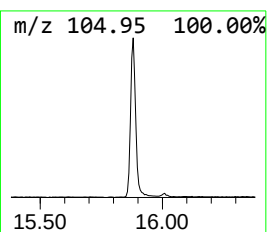
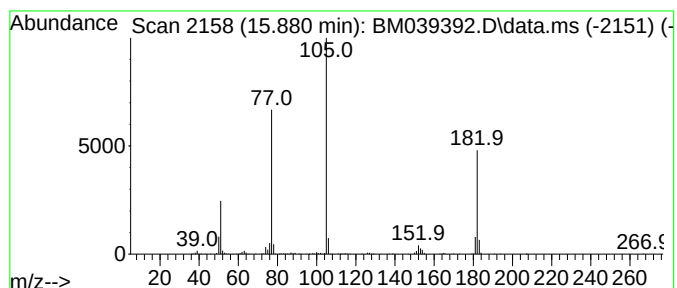
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	5.03 ng	448876	Acenaphthene-d10	14.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5			Benzilic acid	228	C14H12O3	000076-93-7	47



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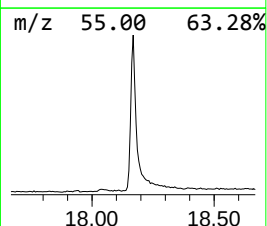
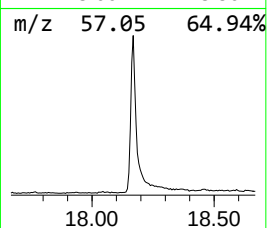
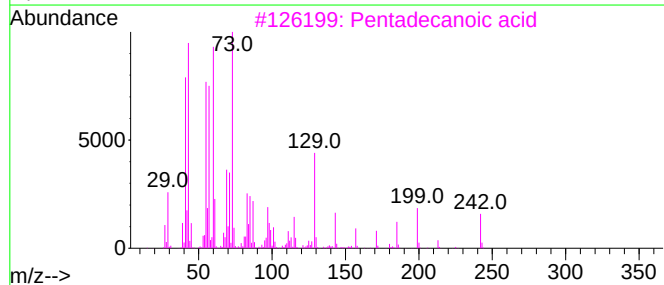
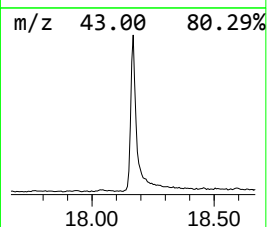
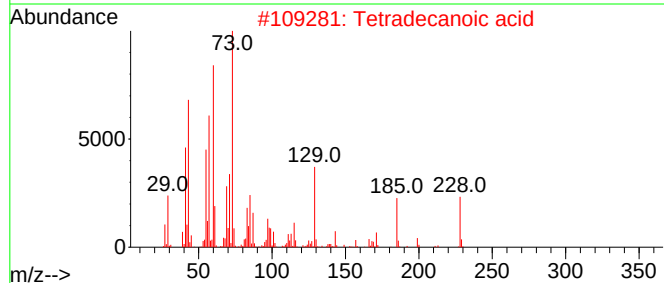
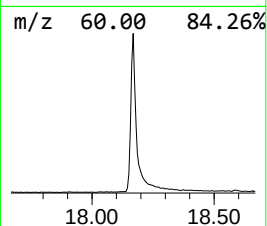
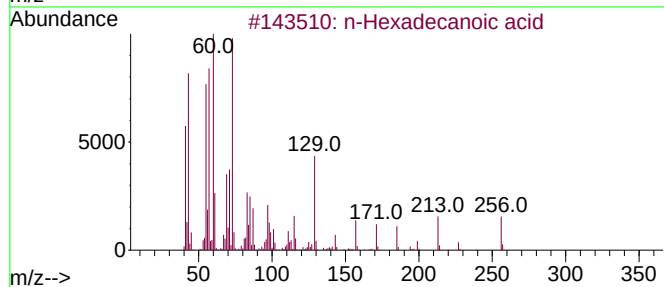
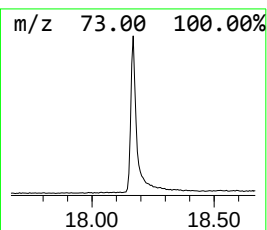
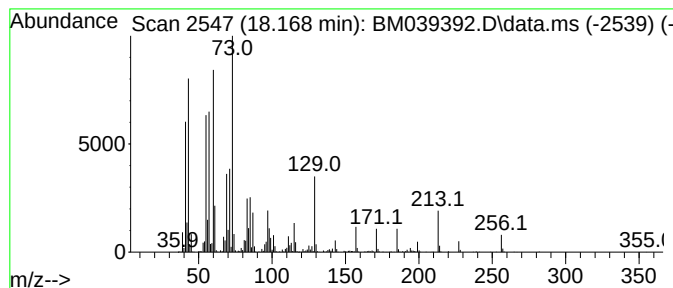
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.168	21.84 ng	2243000	Phenanthrene-d10	17.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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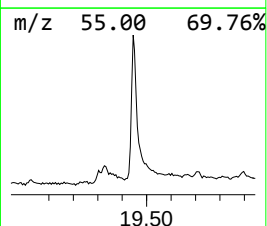
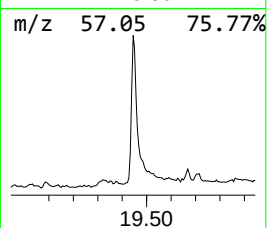
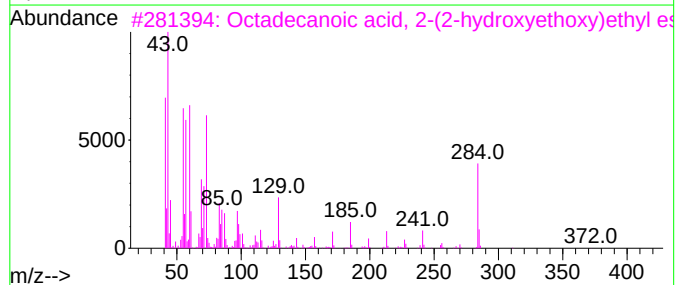
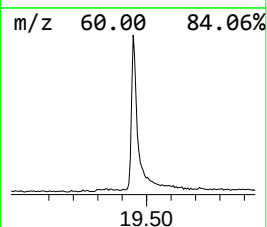
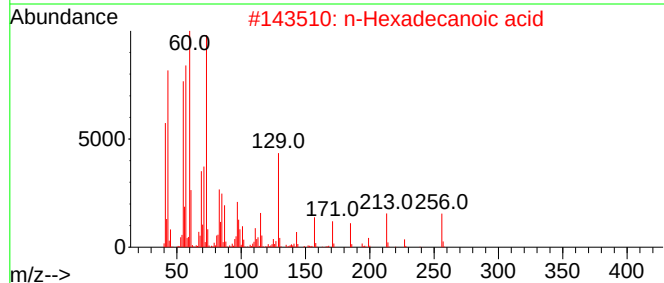
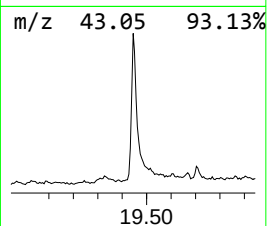
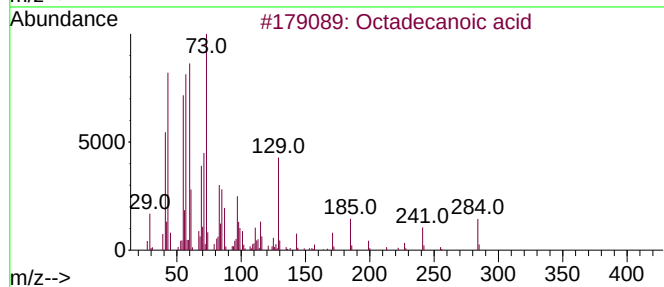
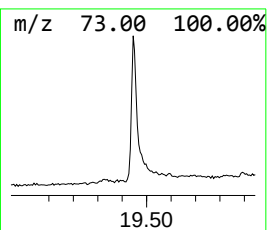
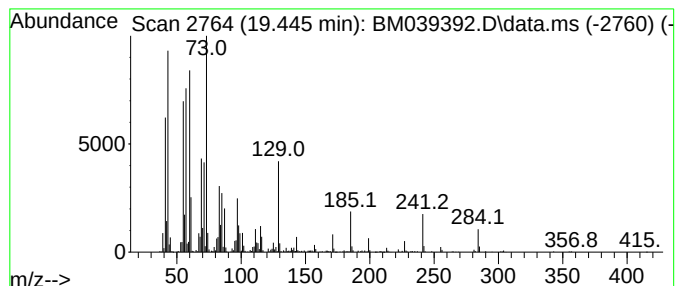
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	6.46 ng	1067930	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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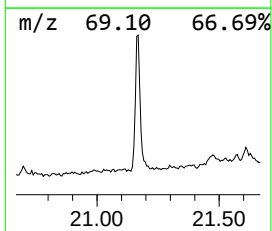
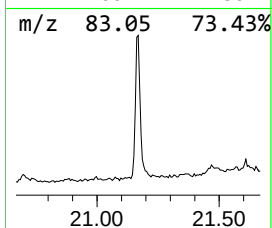
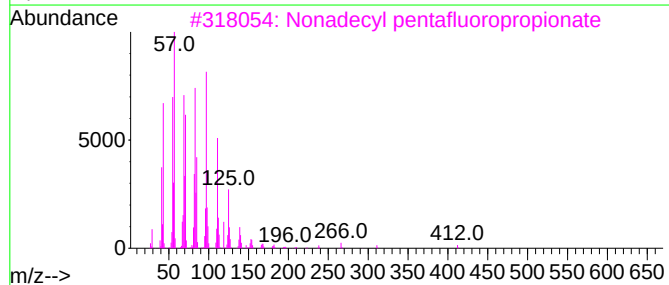
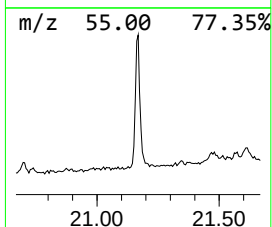
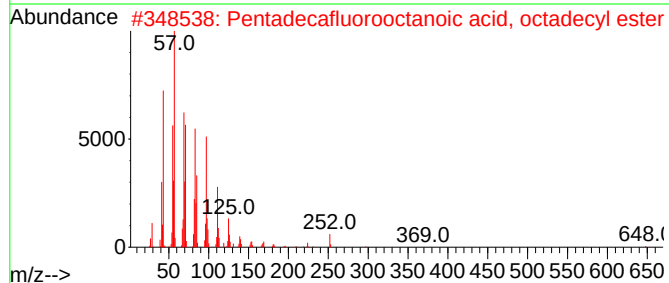
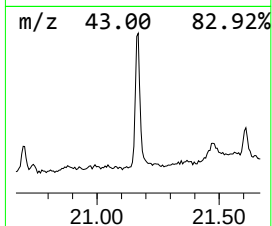
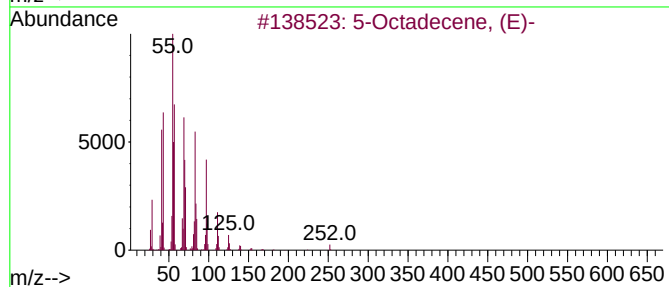
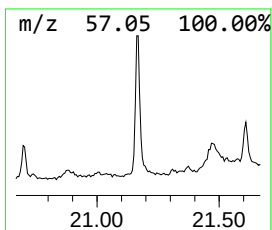
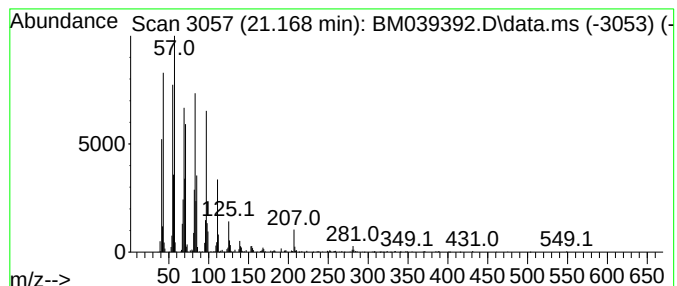
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.168	4.68 ng	773525	Chrysene-d12	21.462

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5		Nonacos-1-ene	406	C29H58	018835-35-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041123\
Data File : BM039392.D
Acq On : 11 Apr 2023 13:46
Operator : CG/JU
Sample : 02256-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
360

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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-...	4.951	25.8	ng	1255210	1	7.863	971630	20.0
3-(2-Hydroxyeth...	13.457	2.3	ng	201912	3	14.515	1786090	20.0
Benzophenone	15.880	5.0	ng	448876	3	14.515	1786090	20.0
n-Hexadecanoic ...	18.168	21.8	ng	2243000	4	17.268	2054480	20.0
Octadecanoic acid	19.445	6.5	ng	1067930	5	21.462	3306790	20.0
5-Octadecene, (E)-	21.168	4.7	ng	773525	5	21.462	3306790	20.0