

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
 Data File : BM039144.D
 Acq On : 24 Mar 2023 16:35
 Operator : CG/JU
 Sample : 02047-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 R-PIT

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-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	291	298	308	rVB	1864414	2553271	24.68%	3.903%
2	5.510	372	378	386	rBV	3995839	5606620	54.20%	8.571%
3	7.116	642	651	665	rBV	3707145	5881008	56.85%	8.990%
4	7.951	784	793	800	rBV	911075	1437085	13.89%	2.197%
5	9.122	984	992	999	rBV	2353474	3829897	37.02%	5.855%
6	10.763	1262	1271	1278	rBV	1197351	1992898	19.27%	3.046%
7	13.222	1681	1689	1696	rBV	5443647	8064921	77.97%	12.329%
8	14.592	1913	1922	1929	rBV	1678737	2491572	24.09%	3.809%
9	14.998	1985	1991	1997	rBV3	58888	118605	1.15%	0.181%
10	15.951	2142	2153	2158	rBV	278615	417715	4.04%	0.639%
11	16.080	2168	2175	2183	rBV	4227944	5890570	56.95%	9.005%
12	16.321	2207	2216	2221	rBV2	97672	202529	1.96%	0.310%
13	17.339	2383	2389	2394	rBV	2017798	2856365	27.61%	4.366%
14	17.380	2394	2396	2401	rVB	117974	133452	1.29%	0.204%
15	18.233	2534	2541	2552	rBV	1766396	2890063	27.94%	4.418%
16	18.521	2585	2590	2594	rBV2	80072	127232	1.23%	0.194%
17	18.657	2609	2613	2618	rBV	441767	493171	4.77%	0.754%
18	19.392	2734	2738	2745	rVB2	218878	308830	2.99%	0.472%
19	19.509	2753	2758	2775	rBV	909206	1519837	14.69%	2.323%
20	19.757	2798	2800	2808	rVB	124843	176562	1.71%	0.270%
21	19.962	2829	2835	2840	rBV	8188705	10344215	100.00%	15.813%
22	20.645	2948	2951	2958	rVB	452906	517295	5.00%	0.791%
23	20.756	2968	2970	2974	rVB2	117128	130246	1.26%	0.199%
24	21.221	3045	3049	3058	rBV	775767	974068	9.42%	1.489%
25	21.521	3095	3100	3104	rBV	2333499	3099298	29.96%	4.738%
26	23.945	3507	3512	3530	rVB2	1584236	3358826	32.47%	5.135%

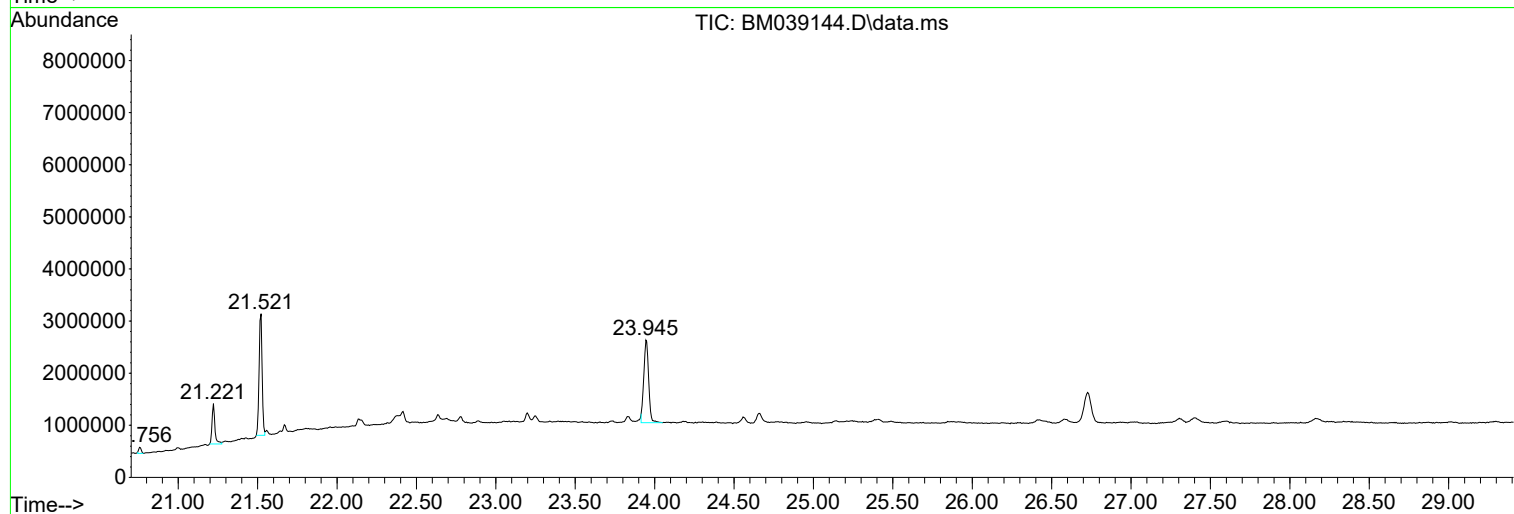
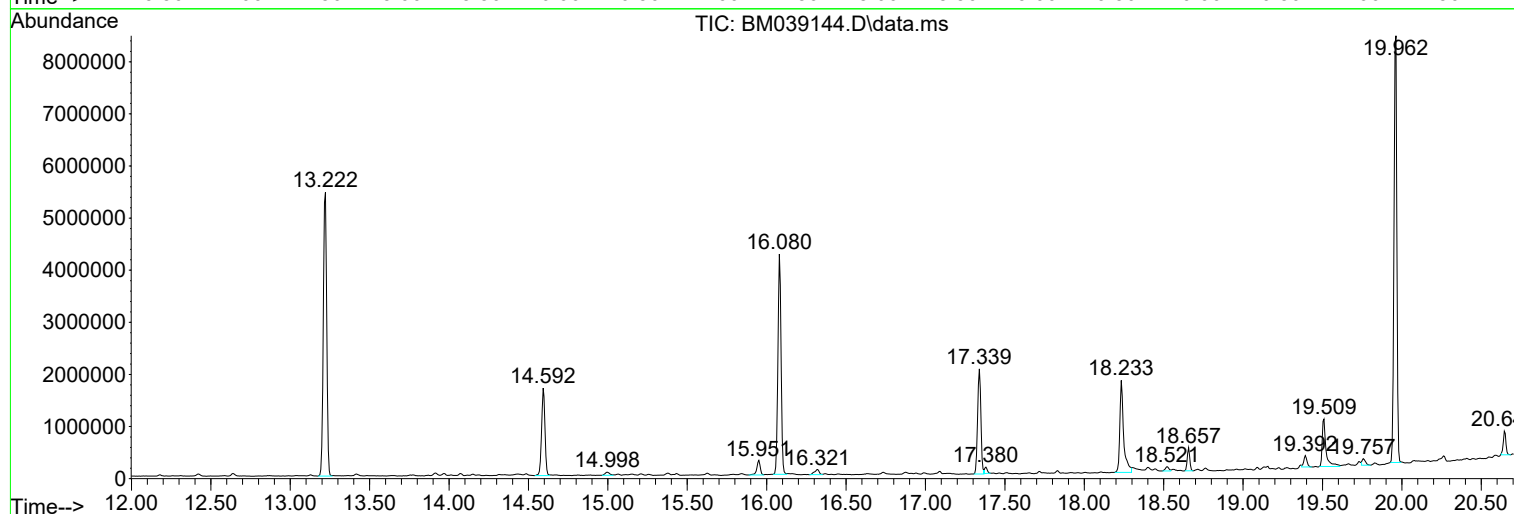
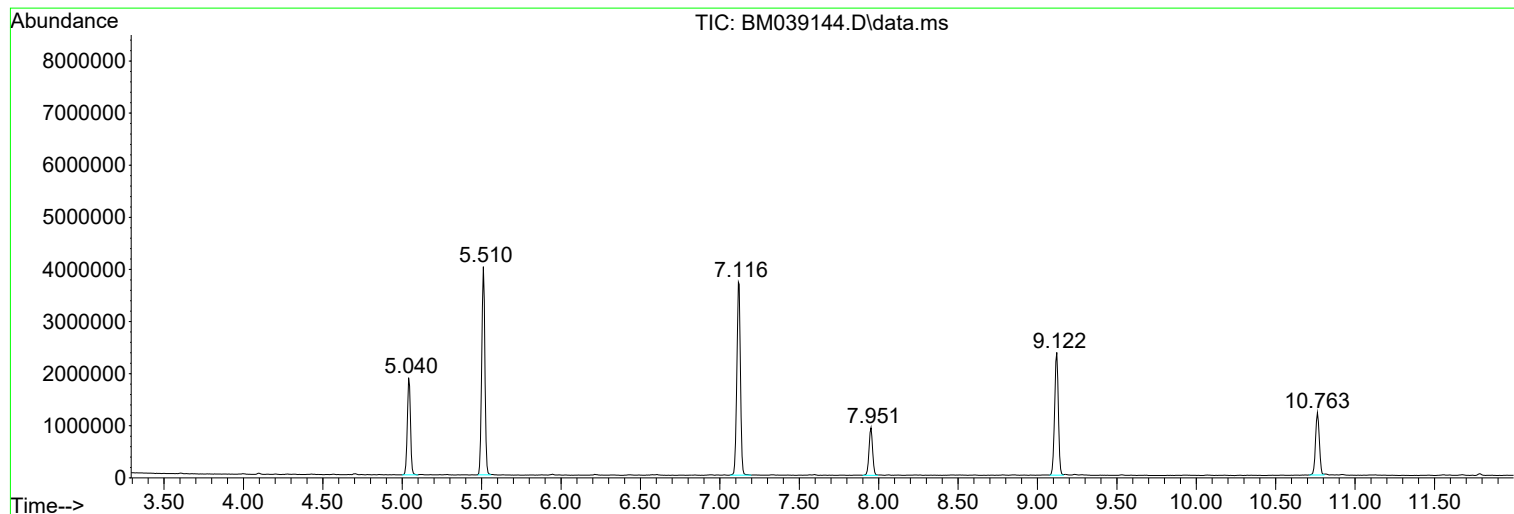
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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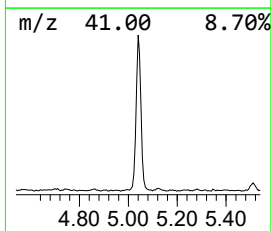
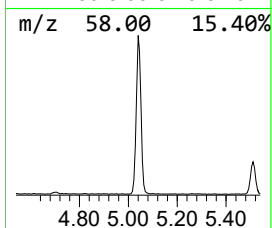
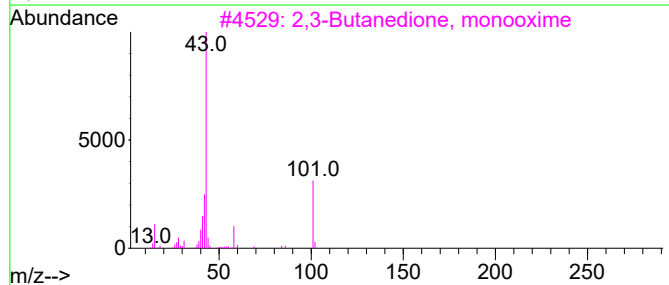
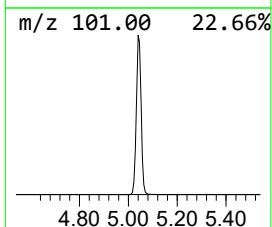
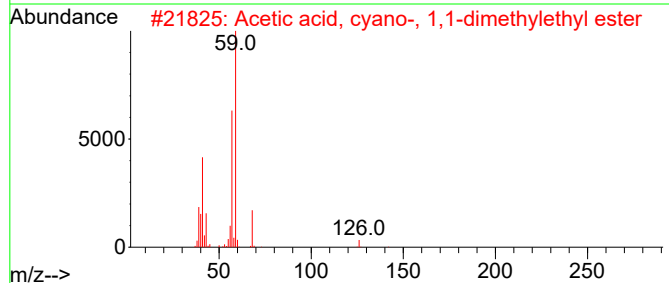
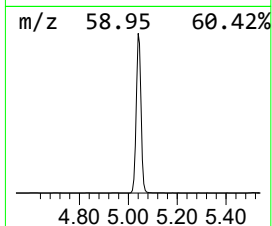
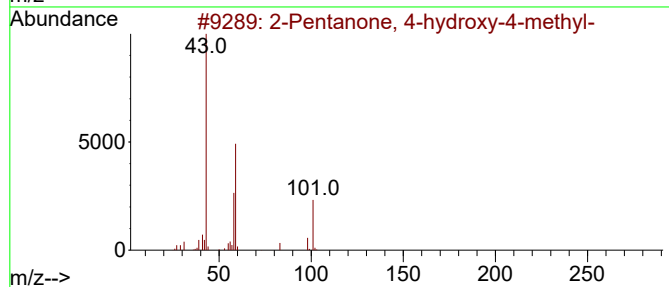
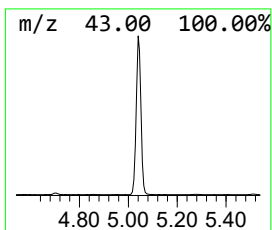
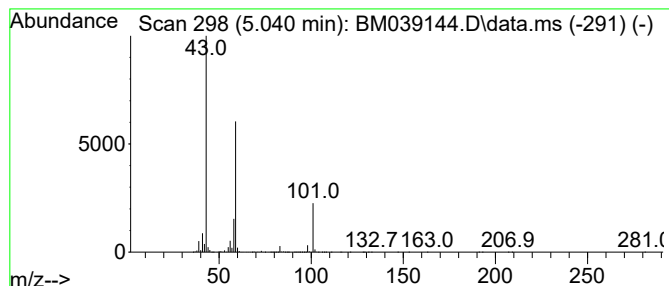
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	35.53 ng	2553270	1,4-Dichlorobenzene-d4	7.951

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	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
4	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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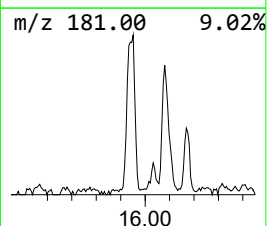
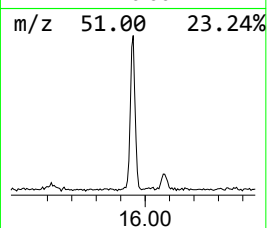
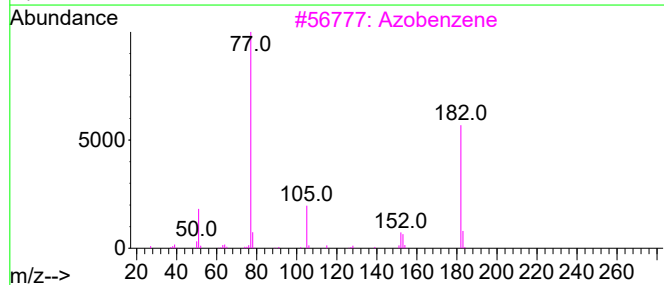
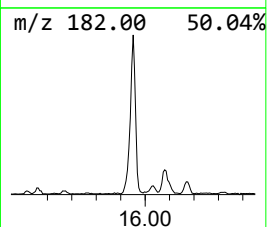
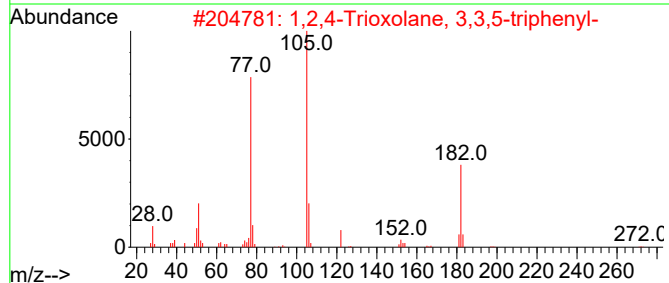
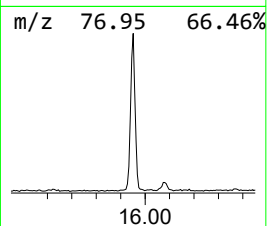
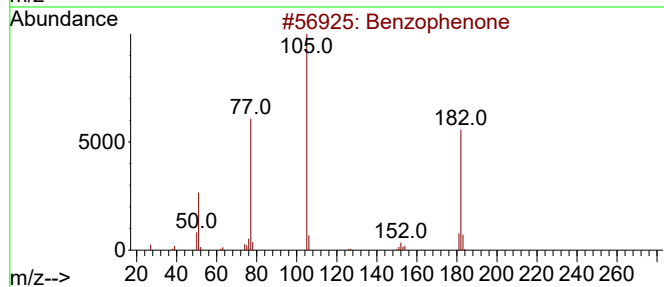
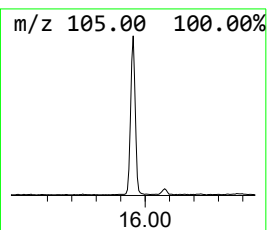
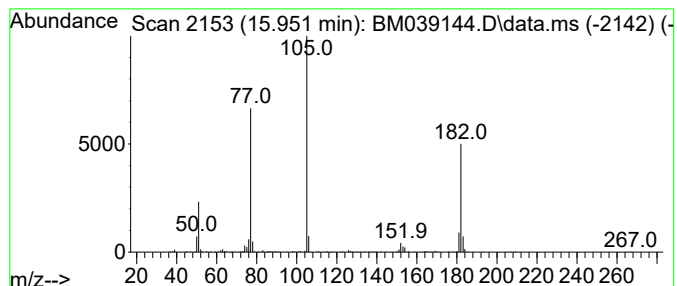
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Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	3.35 ng	417715	Acenaphthene-d10	14.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3			Azobenzene	182	C12H10N2	000103-33-3	58
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



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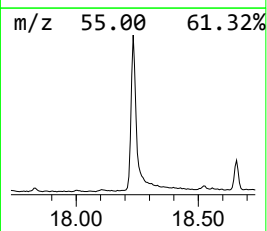
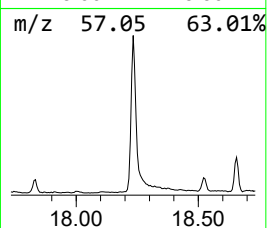
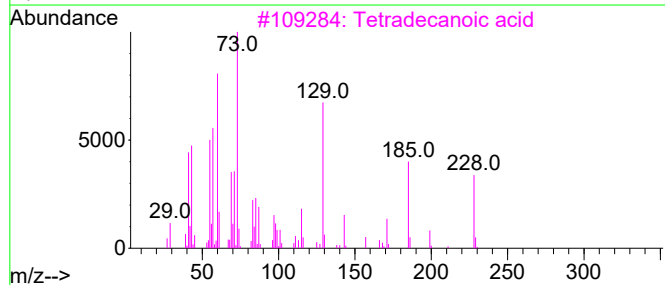
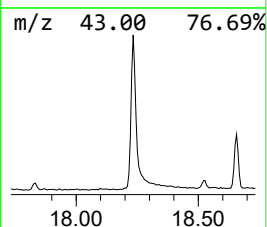
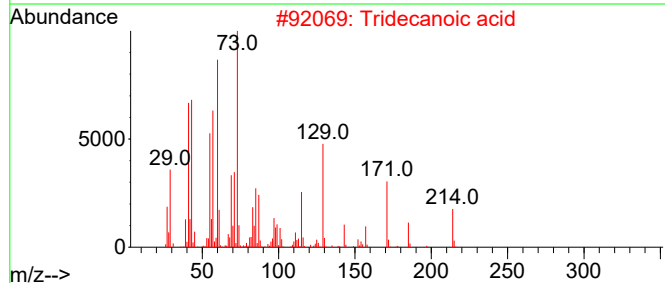
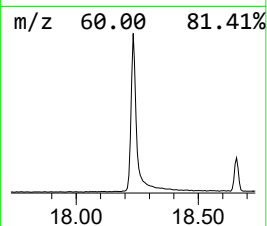
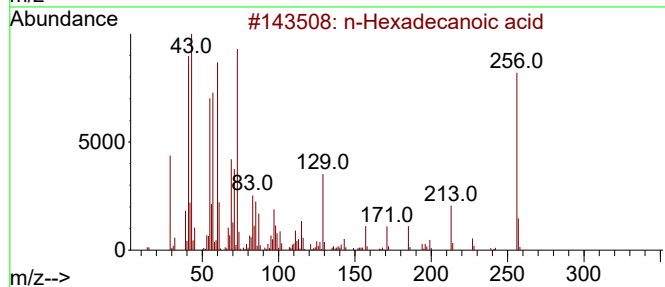
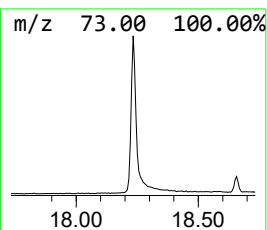
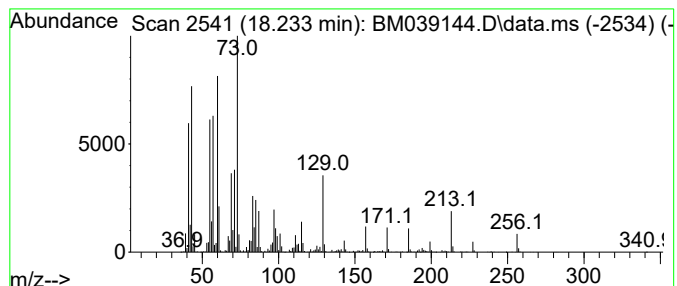
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	20.24 ng	2890060	Phenanthrene-d10	17.339

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46



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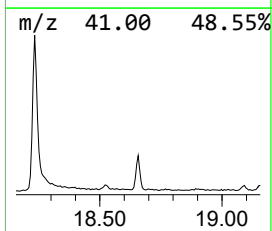
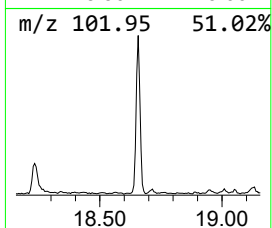
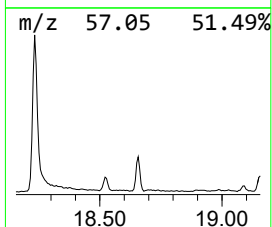
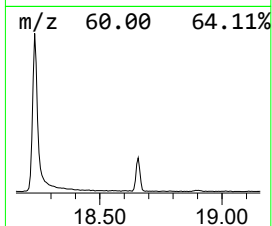
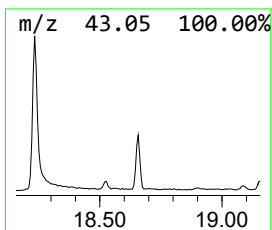
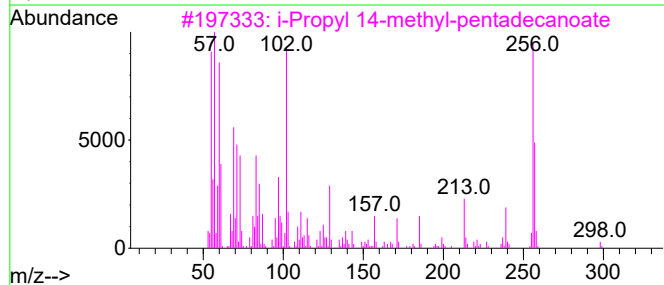
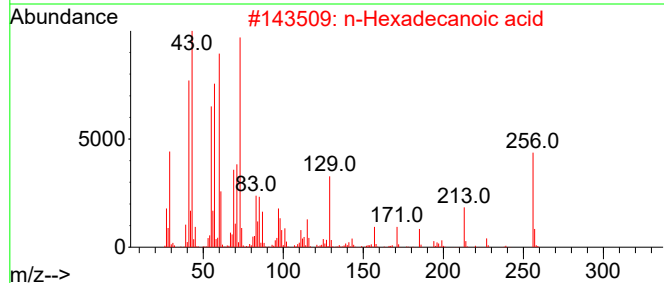
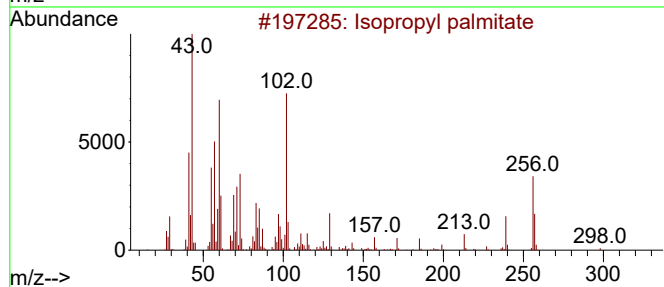
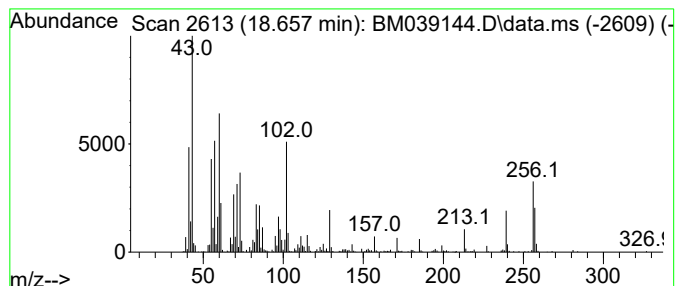
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Peak Number 4 Isopropyl palmitate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.657	3.45 ng	493171	Phenanthrene-d10	17.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	90
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	84
3			i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	83
4			Undecanoic acid	186	C11H22O2	000112-37-8	27
5			Urea, (2-thiazolin-2-yl)-	145	C4H7N3OS	015823-99-1	12



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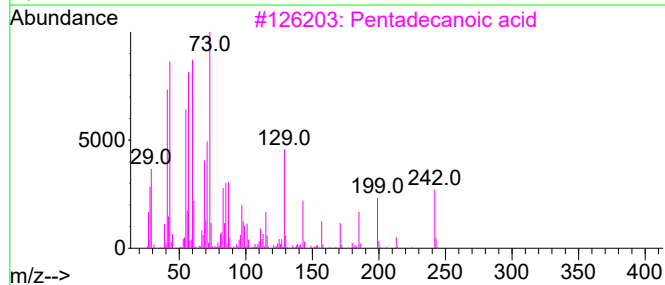
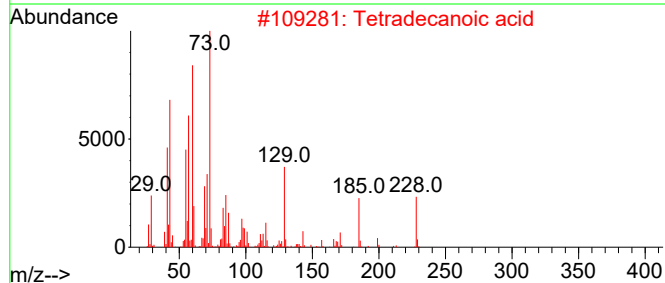
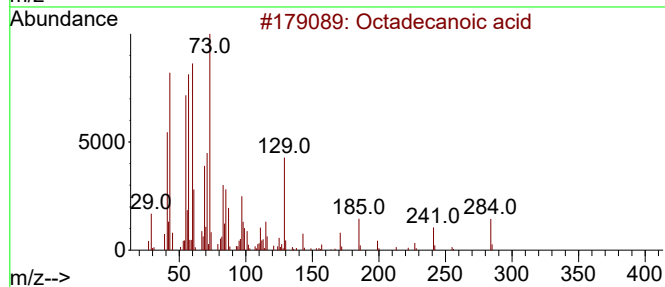
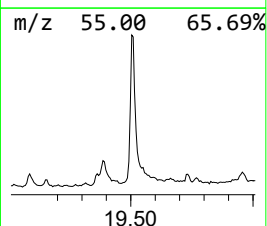
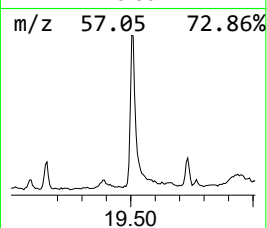
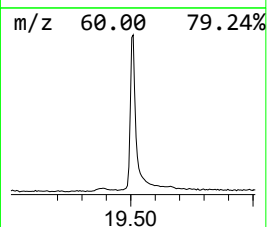
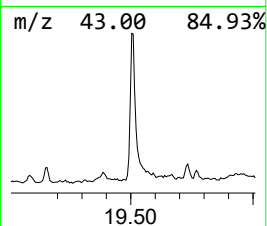
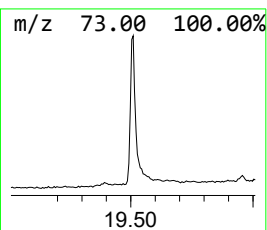
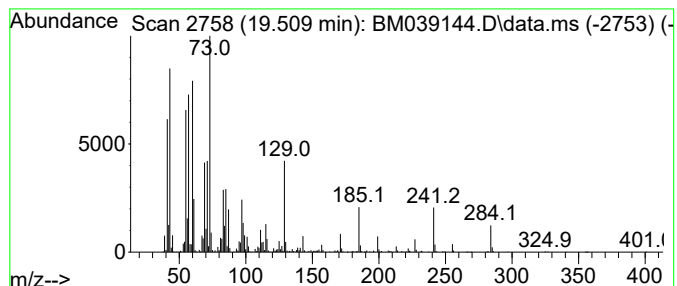
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Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	9.81 ng	1519840	Chrysene-d12	21.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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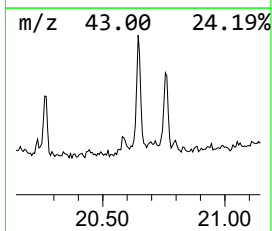
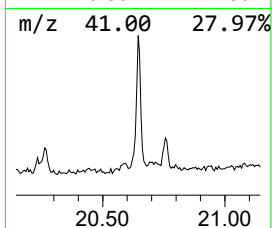
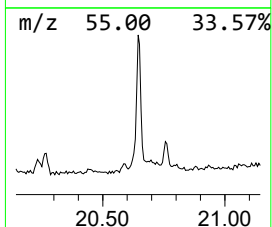
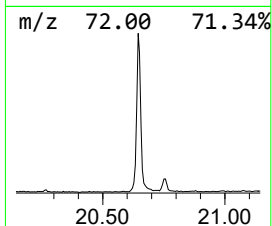
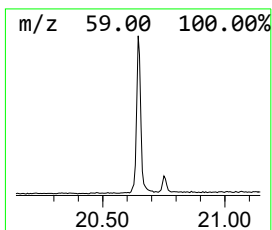
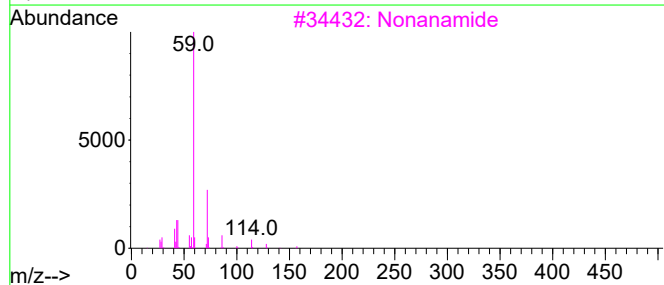
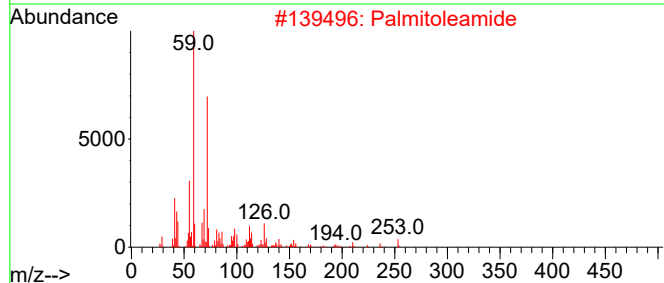
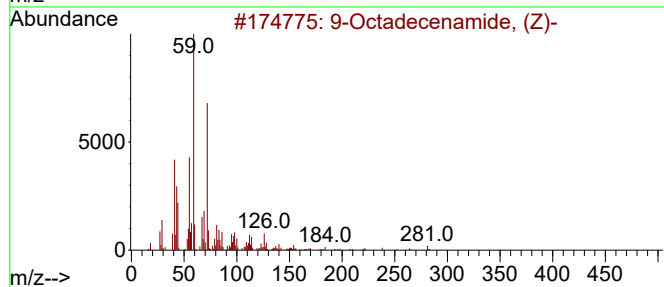
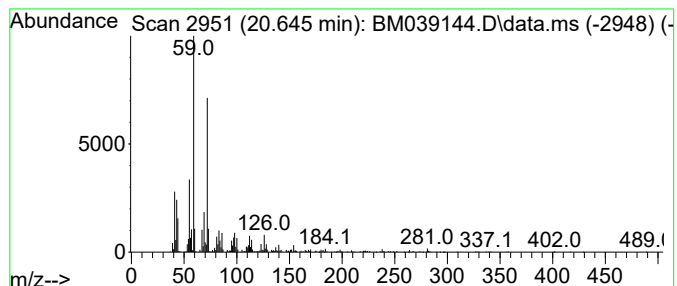
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.645	3.34 ng	517295	Chrysene-d12	21.521

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		Palmitoleamide	253	C16H31NO	106010-22-4	80
3		Nonanamide	157	C9H19NO	001120-07-6	64
4		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	60
5		Hexadecanamide	255	C16H33NO	000629-54-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039144.D
Acq On : 24 Mar 2023 16:35
Operator : CG/JU
Sample : 02047-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
R-PIT

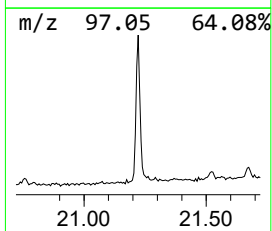
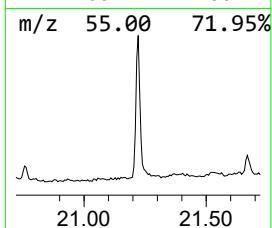
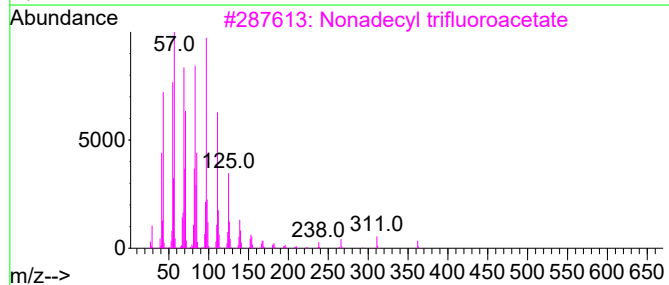
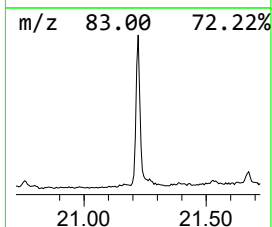
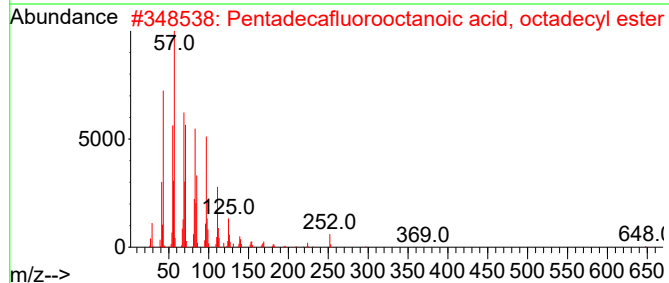
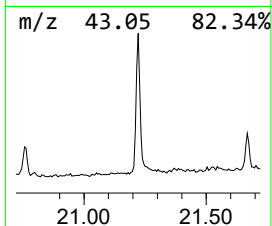
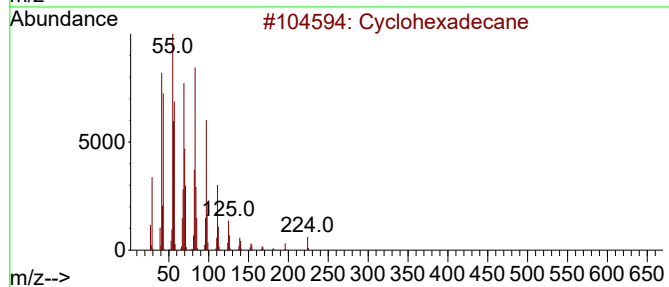
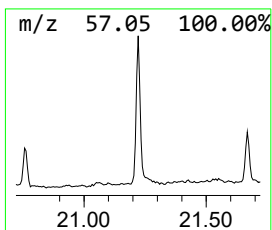
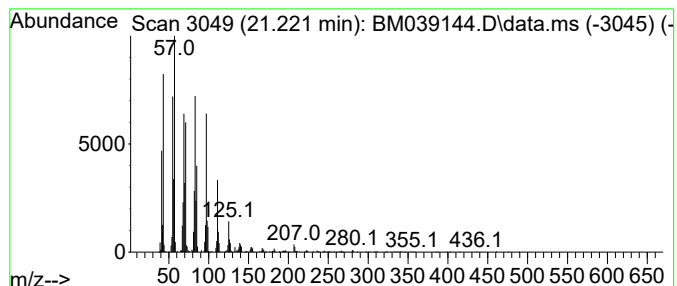
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	6.29 ng	974068	Chrysene-d12	21.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039144.D
Acq On : 24 Mar 2023 16:35
Operator : CG/JU
Sample : 02047-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
R-PIT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.040	35.5	ng	2553270	1	7.951	1437090	20.0
Benzophenone	15.951	3.4	ng	417715	3	14.592	2491570	20.0
n-Hexadecanoic ...	18.233	20.2	ng	2890060	4	17.339	2856370	20.0
Isopropyl palmi...	18.657	3.5	ng	493171	4	17.339	2856370	20.0
Octadecanoic acid	19.509	9.8	ng	1519840	5	21.521	3099300	20.0
9-Octadecenamid...	20.645	3.3	ng	517295	5	21.521	3099300	20.0
Cyclohexadecane	21.221	6.3	ng	974068	5	21.521	3099300	20.0