

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
 Data File : BM047437.D
 Acq On : 04 Sep 2024 14:04
 Operator : RC/JU
 Sample : P3819-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 OCB-CONCRETE

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: BM047437.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.981	181	186	200	rVB	123799	176552	3.00%	0.457%
2	4.557	276	284	295	rBV	1999968	2858976	48.51%	7.398%
3	5.004	355	360	374	rBV	1092846	1674073	28.40%	4.332%
4	6.569	620	626	650	rBV	1267112	2370242	40.21%	6.134%
5	7.340	751	757	767	rBV	635037	989234	16.78%	2.560%
6	8.492	945	953	971	rBV	1139341	2070693	35.13%	5.358%
7	10.092	1218	1225	1242	rBV	696208	1273044	21.60%	3.294%
8	11.980	1539	1546	1560	rBV3	19459	84166	1.43%	0.218%
9	12.604	1645	1652	1675	rBV	2836239	4727185	80.20%	12.233%
10	14.004	1884	1890	1900	rBV	1036833	1627962	27.62%	4.213%
11	14.480	1968	1971	1979	rVB2	46269	75528	1.28%	0.195%
12	15.398	2121	2127	2134	rBV	162636	284665	4.83%	0.737%
13	15.527	2142	2149	2159	rBV	861346	1532612	26.00%	3.966%
14	15.763	2185	2189	2191	rBV4	40690	65082	1.10%	0.168%
15	16.215	2263	2266	2275	rBV3	76000	152256	2.58%	0.394%
16	16.774	2356	2361	2374	rBV	1223816	1876818	31.84%	4.857%
17	16.986	2394	2397	2400	rBV4	52186	62423	1.06%	0.162%
18	17.457	2474	2477	2483	rVB5	158531	208650	3.54%	0.540%
19	17.710	2515	2520	2528	rBV	2584511	3766994	63.91%	9.748%
20	19.009	2736	2741	2752	rBV	1368046	2204705	37.41%	5.705%
21	19.439	2809	2814	2825	rVB	4662356	5894095	100.00%	15.252%
22	20.745	3032	3036	3043	rVB	513367	751951	12.76%	1.946%
23	21.021	3078	3083	3088	rBV	1360898	1890764	32.08%	4.893%
24	23.727	3536	3543	3554	rVB	844746	2025497	34.36%	5.241%

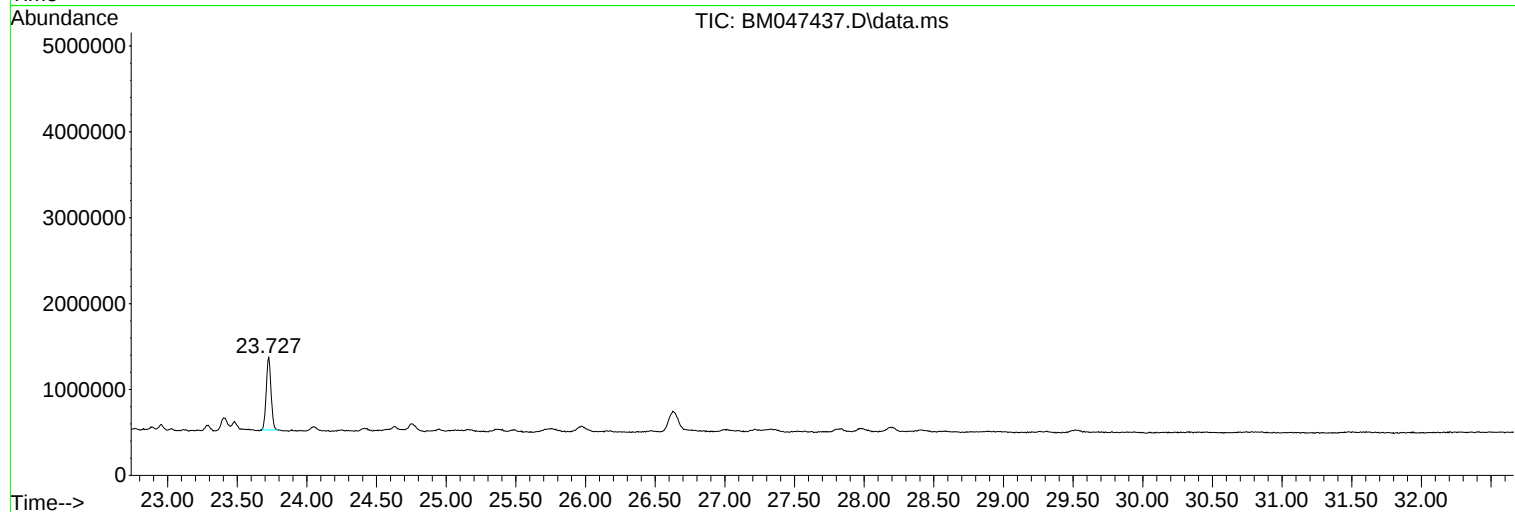
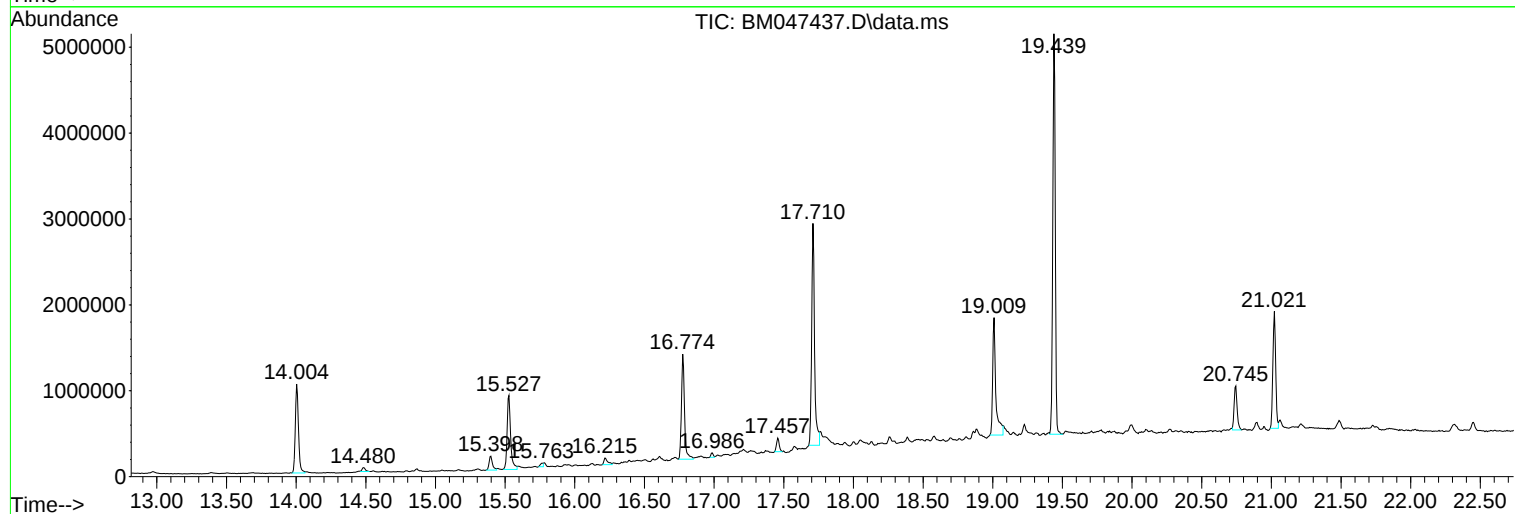
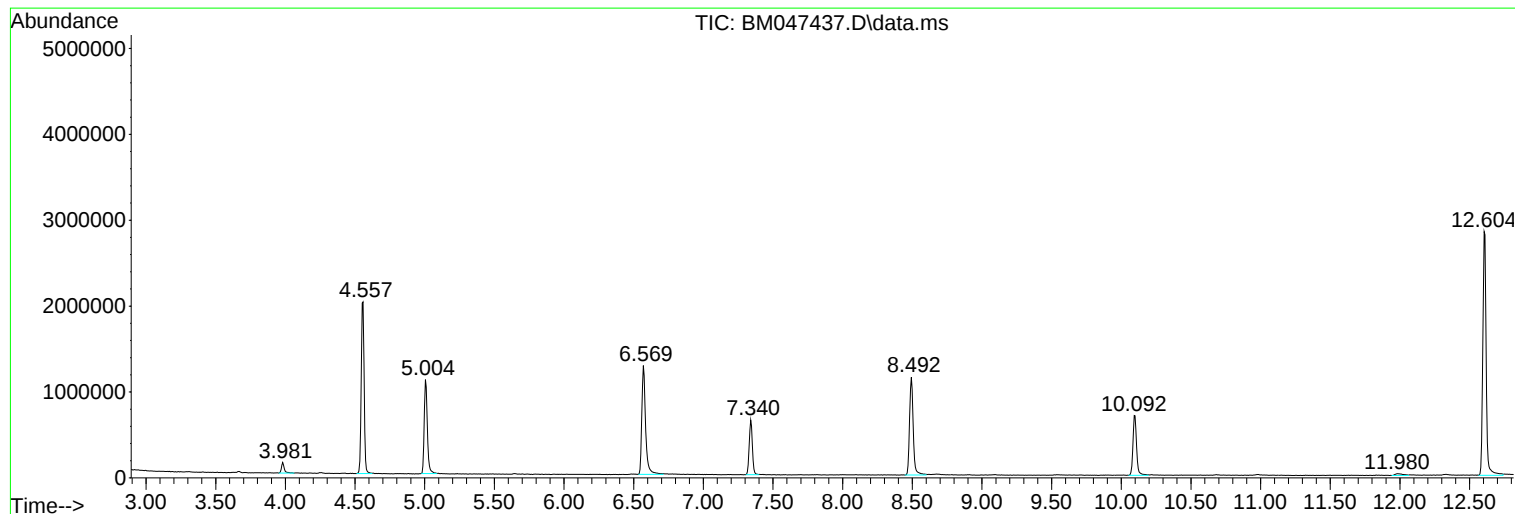
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BNA_M
ClientSampleId :
OCB-CONCRETE

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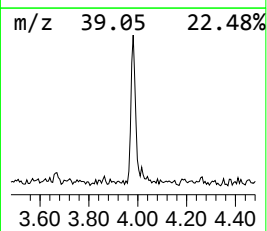
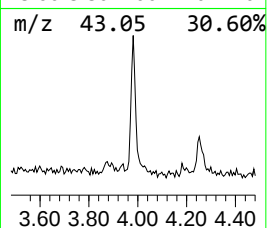
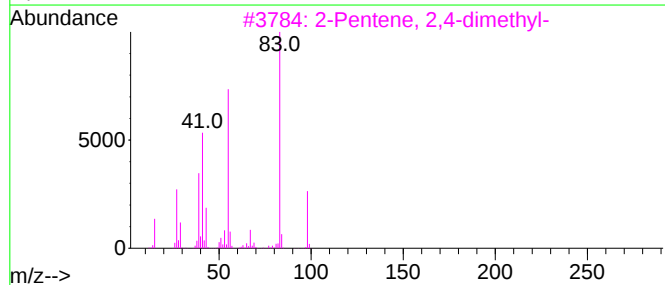
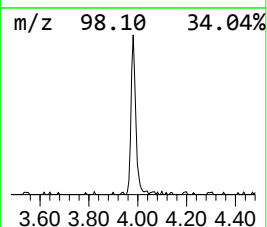
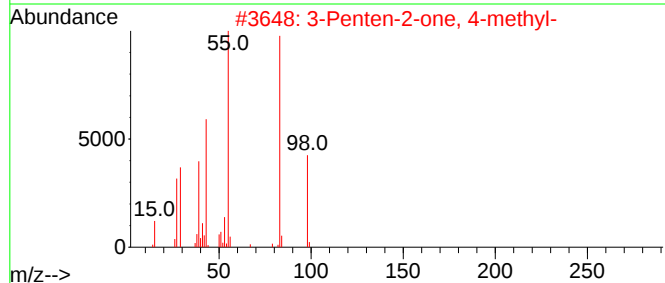
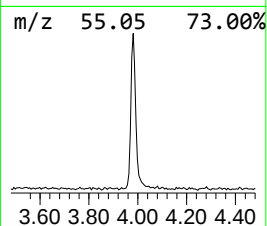
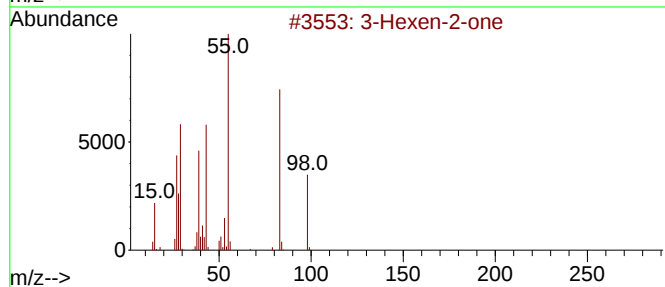
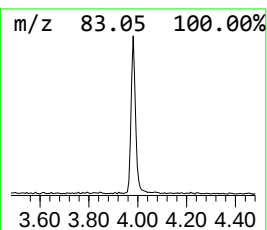
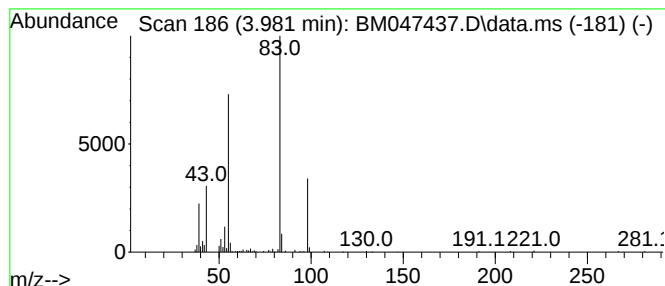
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.981	3.57 ng	176552	1,4-Dichlorobenzene-d4	7.340

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	86



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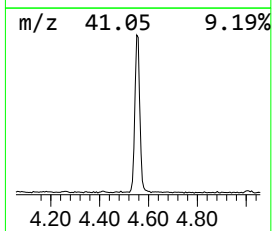
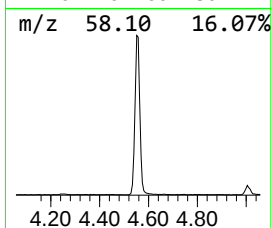
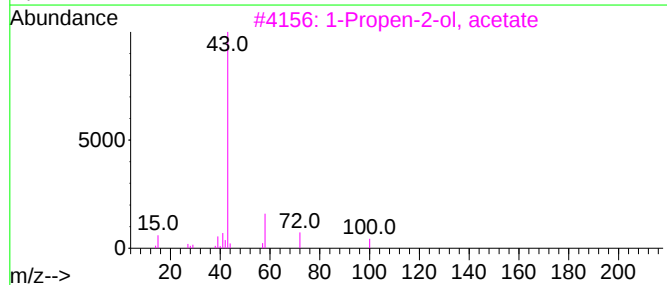
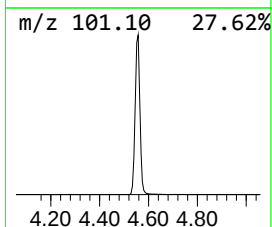
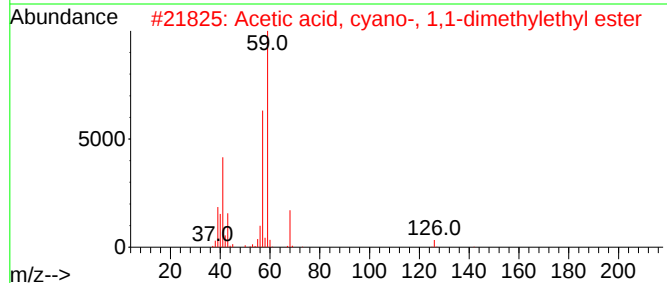
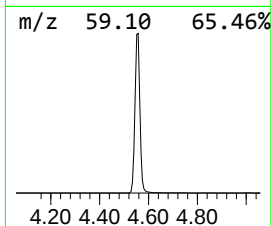
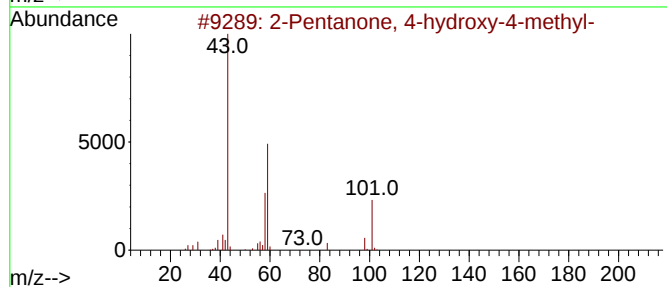
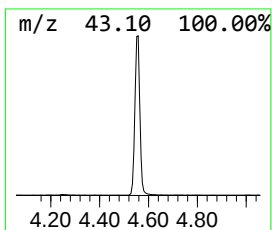
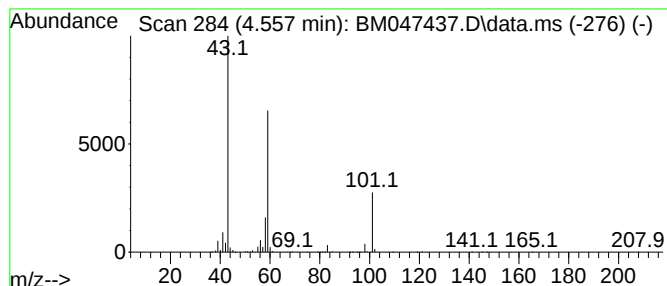
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	57.80 ng	2858980	1,4-Dichlorobenzene-d4	7.340

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	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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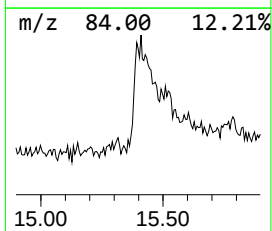
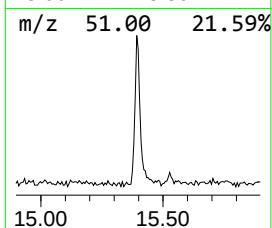
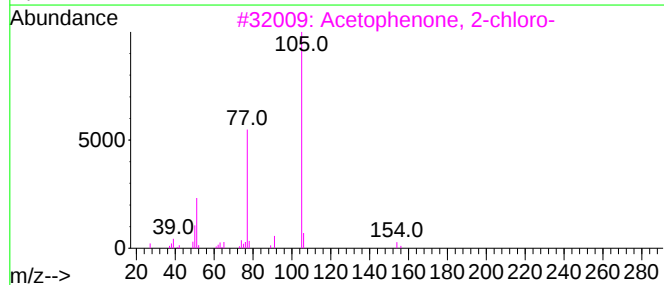
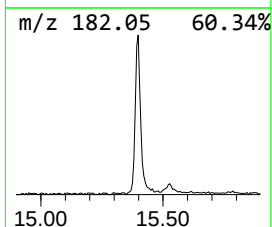
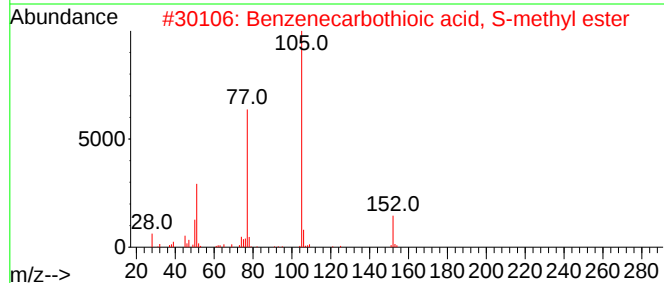
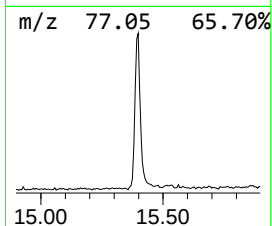
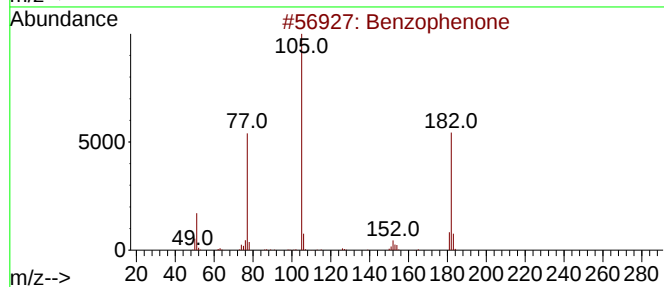
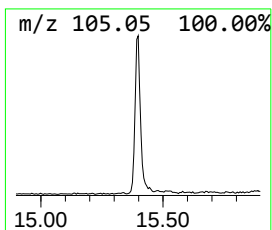
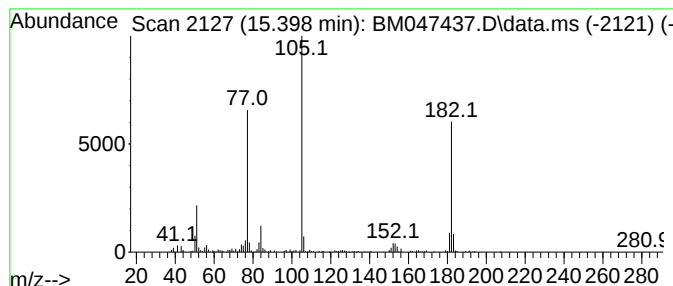
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	3.03 ng	284665	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43



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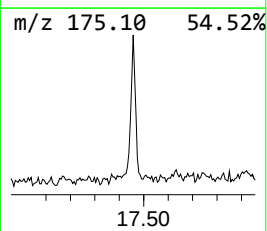
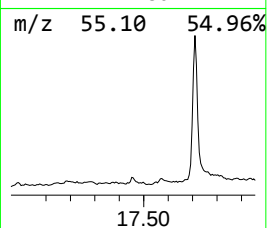
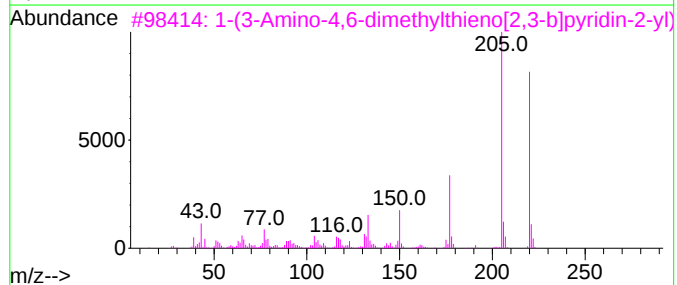
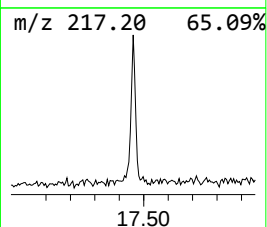
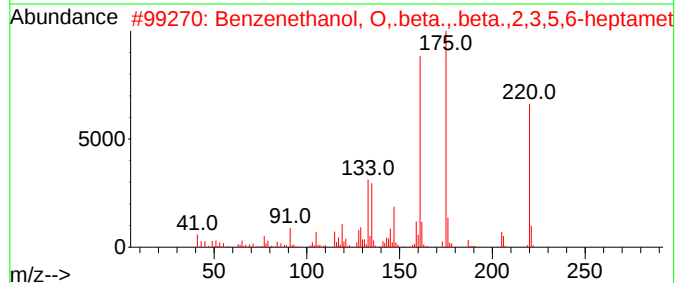
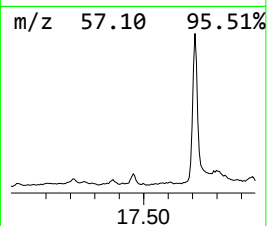
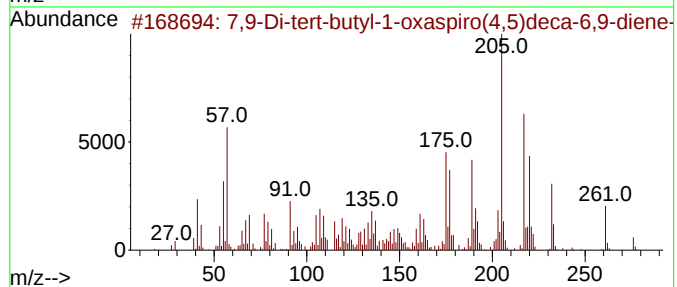
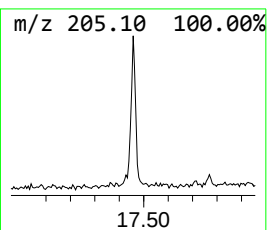
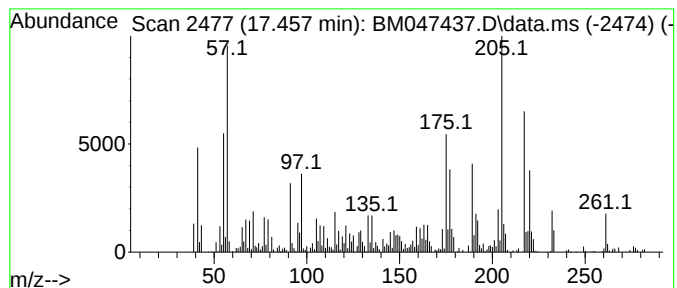
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.457	2.22 ng	208650	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	Benzenethanol, O,.beta.,.beta.,2...	220	C15H24O	1010128-94-8	58		
3	1-(3-Amino-4,6-dimethylthieno[2...	220	C11H12N2OS	052505-42-7	43		
4	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	38		
5	5-Fluoro-2-(1H-imidazol-1-yl)phe...	205	C11H12FN3	1000512-19-0	30		



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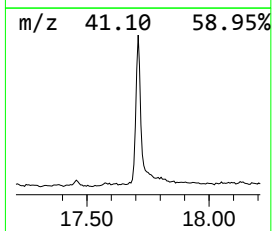
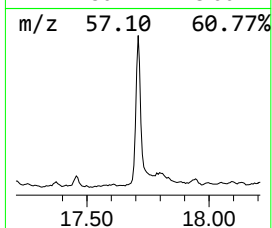
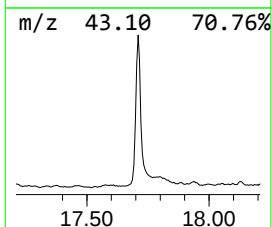
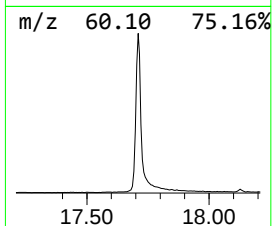
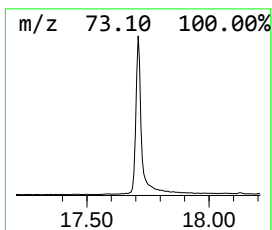
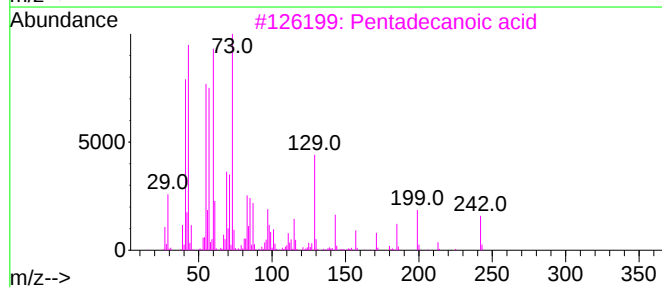
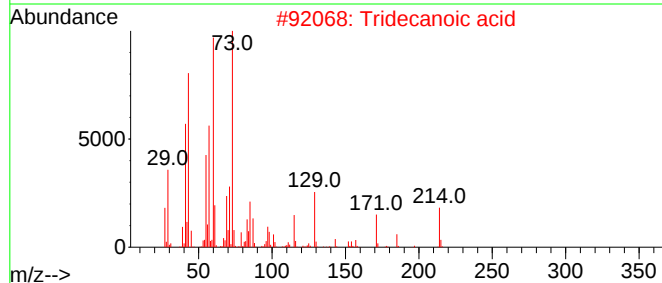
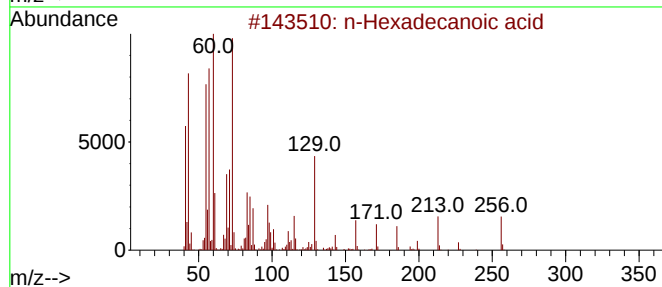
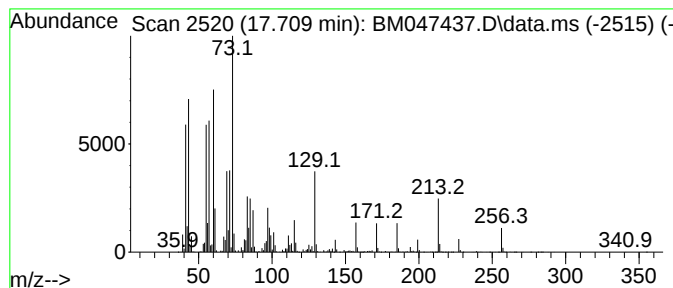
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.709	40.14 ng	3766990	Phenanthrene-d10		16.774	
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	90
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	86
5	n-Decanoic acid		172	C10H20O2	000334-48-5	58



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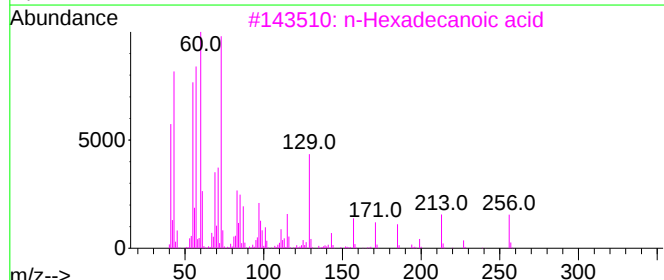
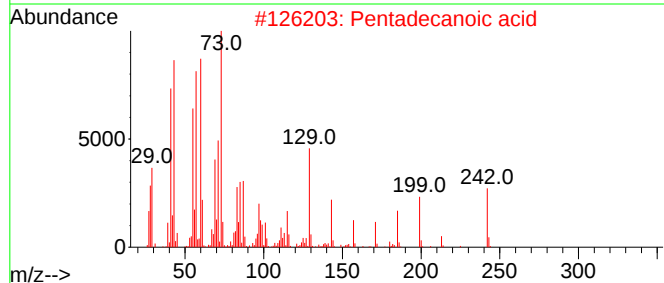
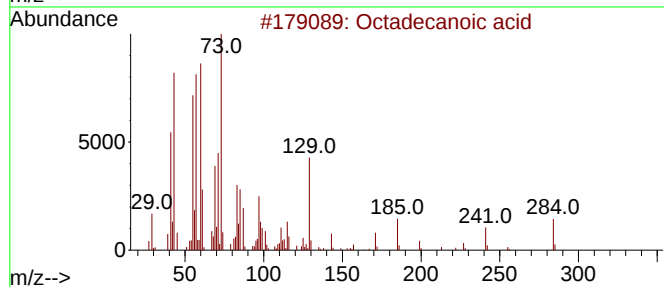
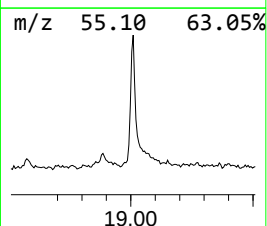
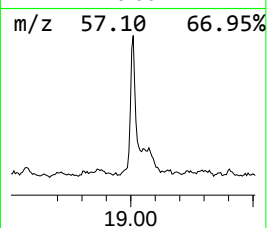
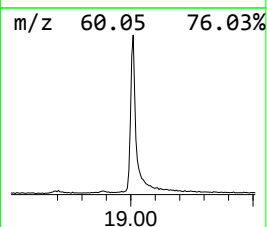
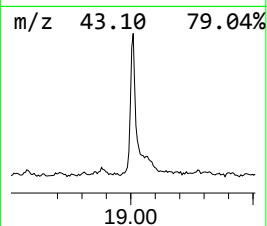
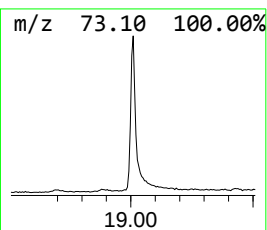
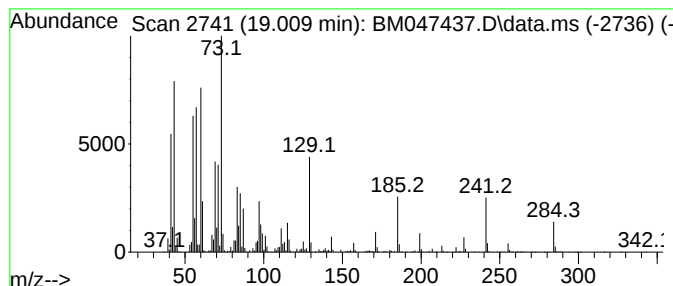
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	23.32 ng	2204710	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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
Data File : BM047437.D
Acq On : 04 Sep 2024 14:04
Operator : RC/JU
Sample : P3819-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OCB-CONCRETE

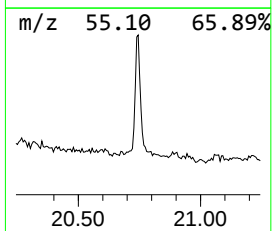
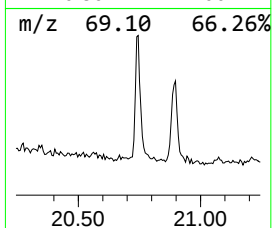
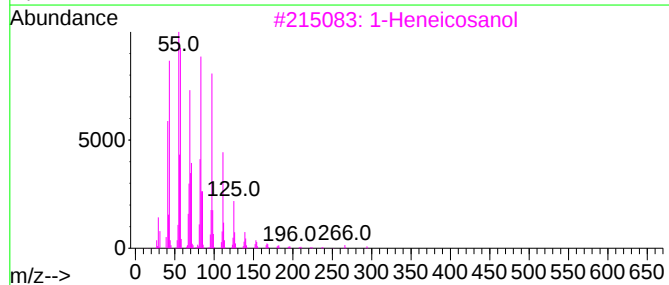
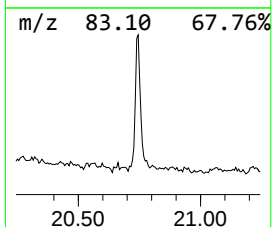
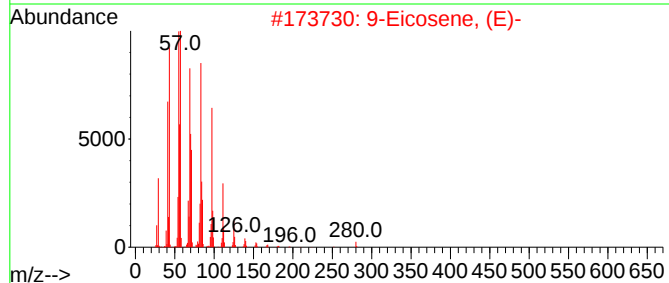
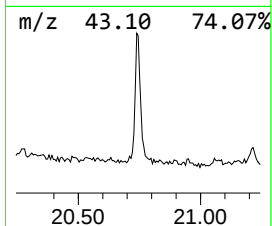
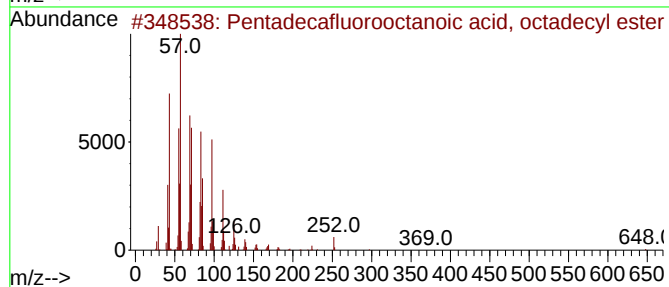
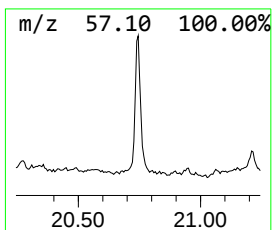
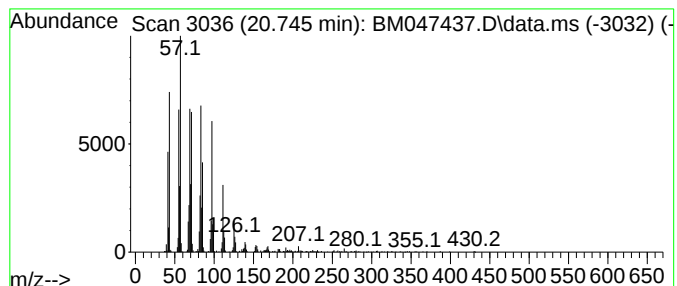
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.745	7.95 ng	751951	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
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\BM090424\
Data File : BM047437.D
Acq On : 04 Sep 2024 14:04
Operator : RC/JU
Sample : P3819-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OCB-CONCRETE

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
3-Hexen-2-one	3.981	3.6	ng	176552	1	7.340	989234	20.0
2-Pentanone, 4-...	4.557	57.8	ng	2858980	1	7.340	989234	20.0
Benzophenone	15.398	3.0	ng	284665	4	16.774	1876820	20.0
7,9-Di-tert-but...	17.457	2.2	ng	208650	4	16.774	1876820	20.0
n-Hexadecanoic ...	17.709	40.1	ng	3766990	4	16.774	1876820	20.0
Octadecanoic acid	19.009	23.3	ng	2204710	5	21.021	1890760	20.0
Pentadecafluoro...	20.745	8.0	ng	751951	5	21.021	1890760	20.0