

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090524\
 Data File : BM047449.D
 Acq On : 05 Sep 2024 16:06
 Operator : RC/JU
 Sample : P3836-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DN-B-38(B-8)

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: BM047449.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	197	rBV	106283	165235	2.22%	0.300%
2	4.551	276	283	296	rBV	419124	625112	8.40%	1.135%
3	5.004	354	360	379	rBV	3315582	5075451	68.16%	9.216%
4	6.569	619	626	654	rBV	2807708	5251612	70.53%	9.536%
5	7.339	749	757	769	rBV	1015735	1624548	21.82%	2.950%
6	8.492	944	953	972	rBV	1903145	3506405	47.09%	6.367%
7	10.092	1217	1225	1242	rBV	1129413	2077607	27.90%	3.773%
8	11.539	1461	1471	1477	rBV	103523	175666	2.36%	0.319%
9	12.604	1645	1652	1682	rBV	4543524	7445854	100.00%	13.521%
10	12.827	1685	1690	1698	rVB	78240	121309	1.63%	0.220%
11	14.004	1884	1890	1911	rBV	1507294	2589295	34.77%	4.702%
12	15.392	2120	2126	2140	rBV	536414	860564	11.56%	1.563%
13	15.521	2142	2148	2168	rBV	3082831	5346284	71.80%	9.708%
14	15.704	2174	2179	2185	rBV2	40082	93560	1.26%	0.170%
15	15.957	2213	2222	2227	rBV	56049	104474	1.40%	0.190%
16	16.215	2262	2266	2273	rBV	57880	96745	1.30%	0.176%
17	16.774	2355	2361	2374	rBV	1616849	2677929	35.97%	4.863%
18	17.709	2514	2520	2541	rBV	1676023	2800234	37.61%	5.085%
19	18.856	2711	2715	2725	rBV	191361	401626	5.39%	0.729%
20	19.003	2736	2740	2753	rBV	518104	900794	12.10%	1.636%
21	19.139	2760	2763	2770	rVB	70610	75705	1.02%	0.137%
22	19.221	2774	2777	2783	rVB	140751	202108	2.71%	0.367%
23	19.439	2808	2814	2824	rBV	5383319	7093983	95.27%	12.882%
24	20.739	3031	3035	3042	rBV2	435827	605015	8.13%	1.099%
25	20.944	3067	3070	3073	rVB	148102	164700	2.21%	0.299%
26	21.015	3077	3082	3088	rBV	1642220	2446644	32.86%	4.443%
27	23.721	3535	3542	3552	rVB	1135399	2542150	34.14%	4.616%

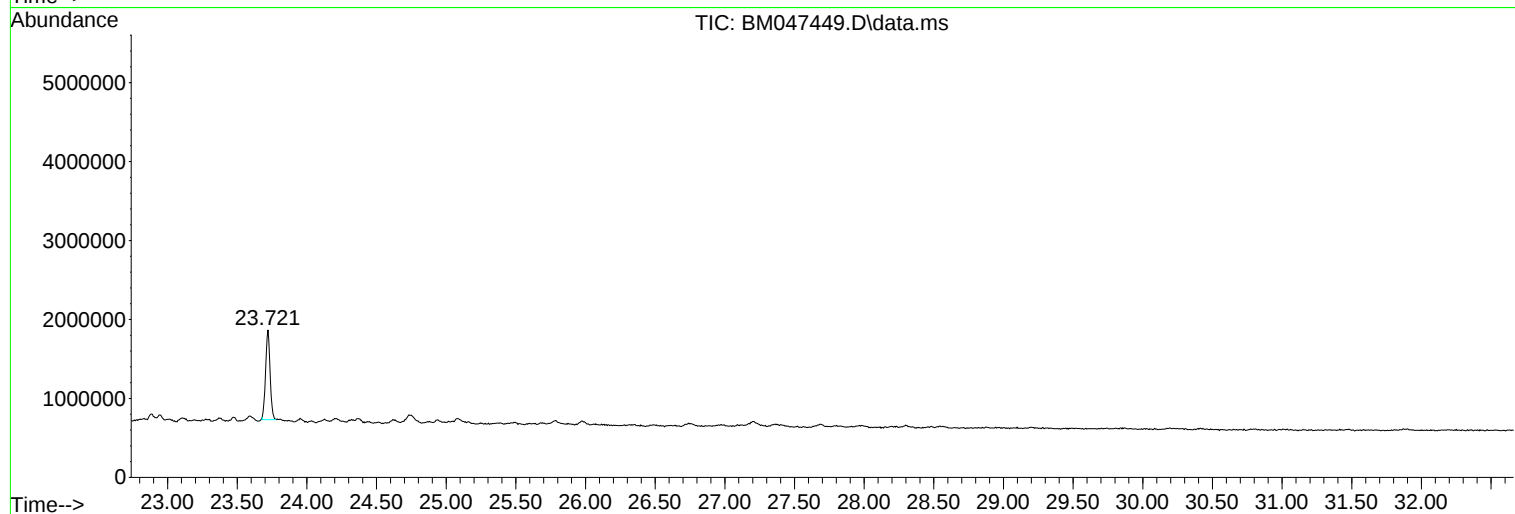
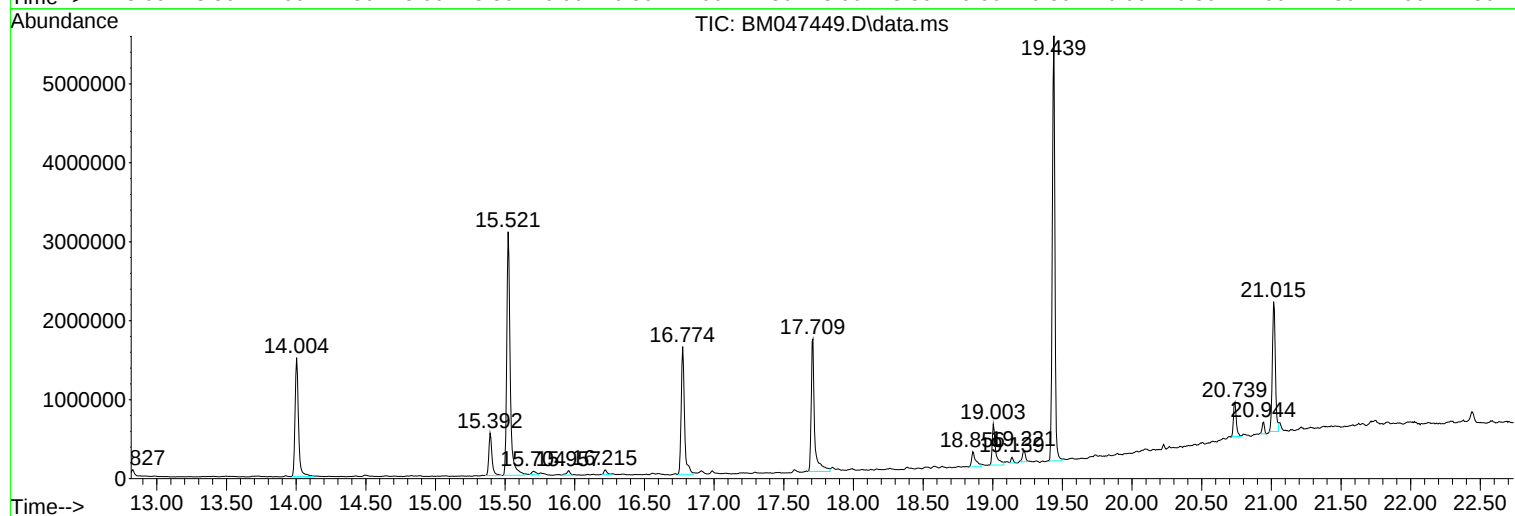
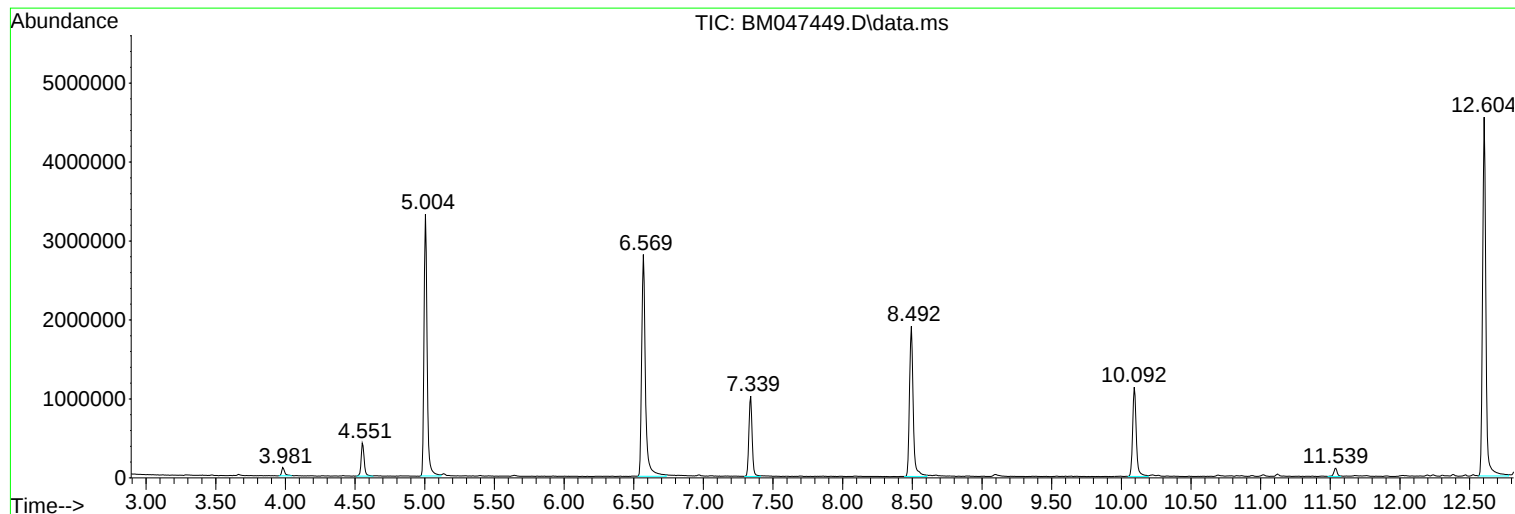
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ClientSampleId :
DN-B-38(B-8)

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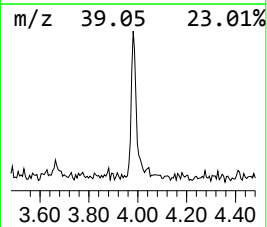
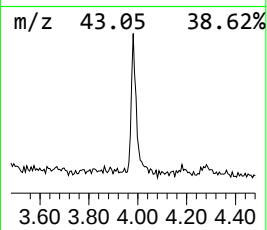
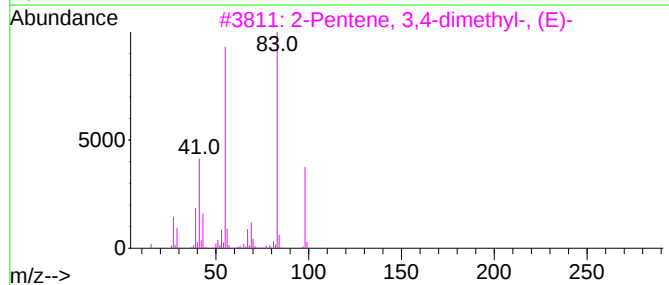
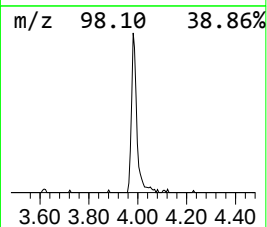
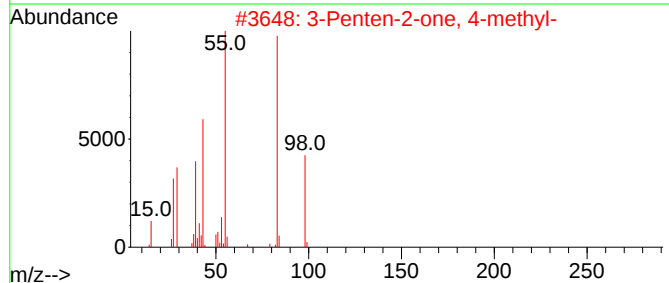
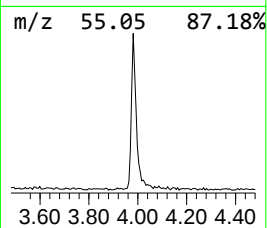
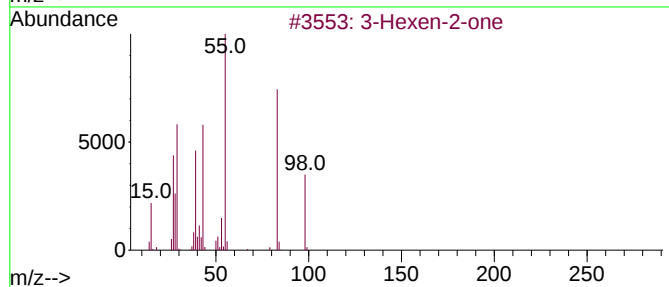
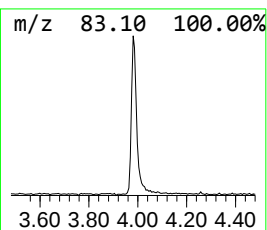
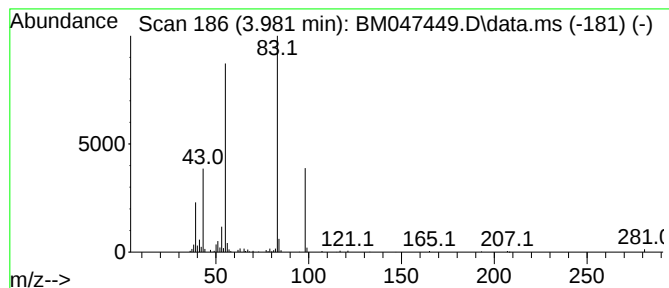
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Hexen-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.981	2.03 ng	165235	1,4-Dichlorobenzene-d4	7.339

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, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	83



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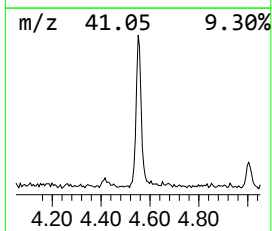
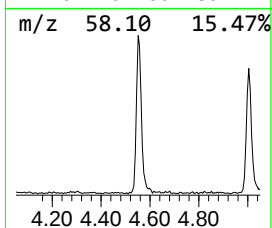
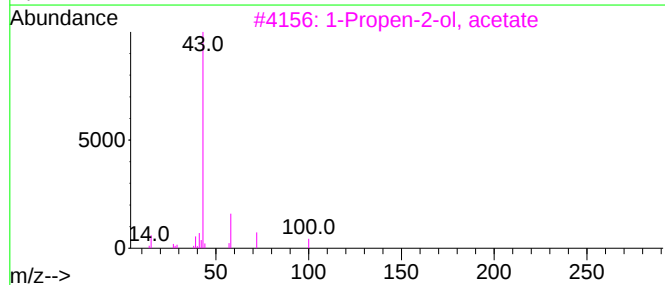
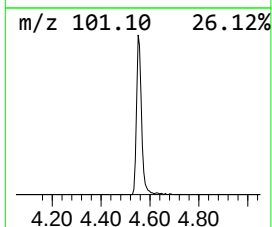
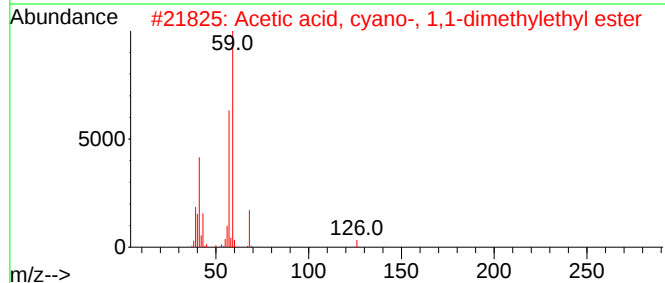
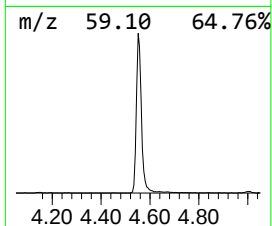
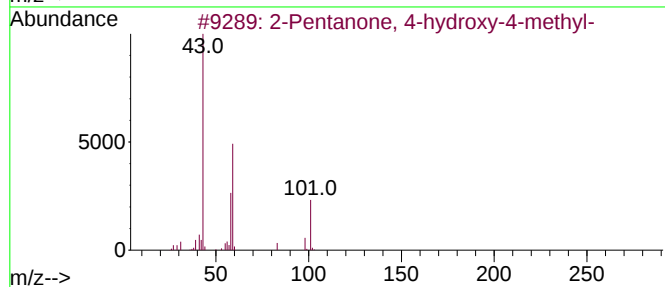
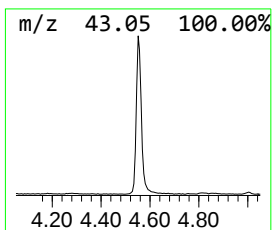
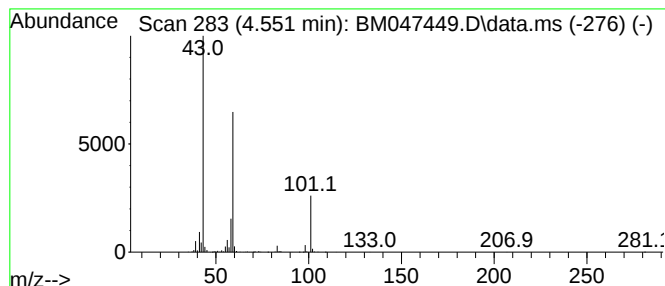
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.551	7.70 ng	625112	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	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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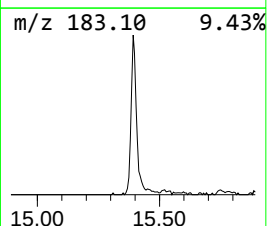
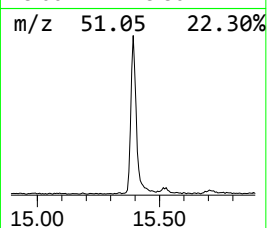
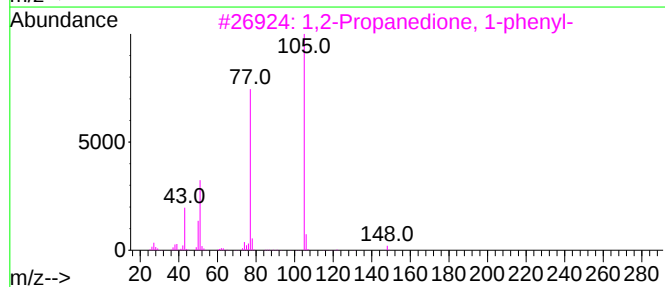
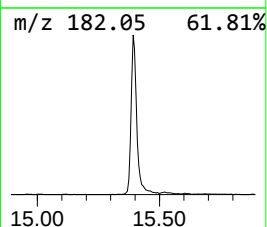
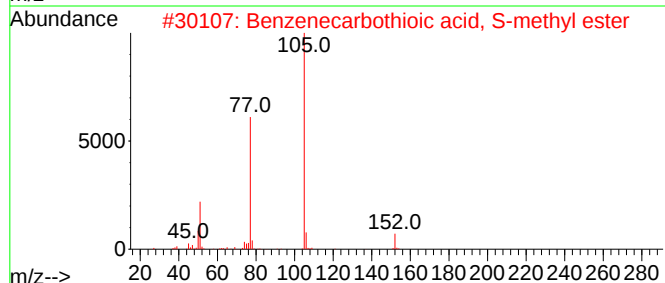
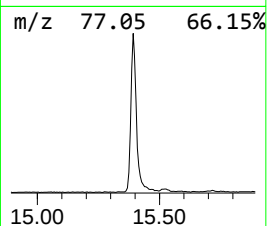
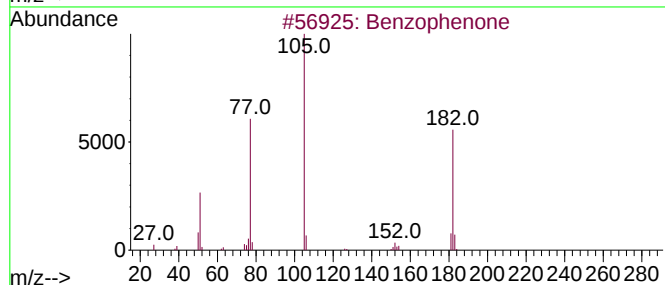
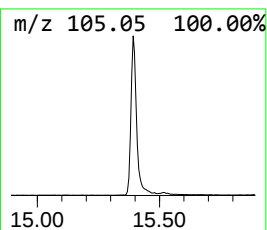
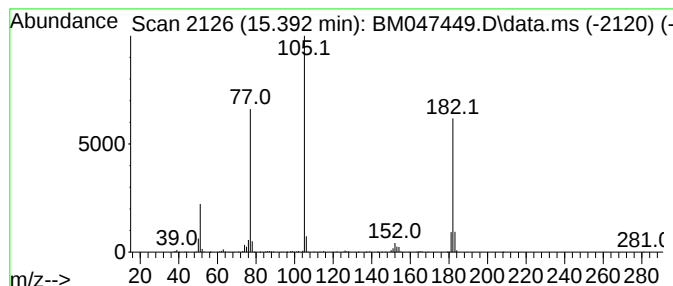
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	6.43 ng	860564	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	47
3			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43
4			Vinyl benzoate	148	C9H8O2	000769-78-8	43
5			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43



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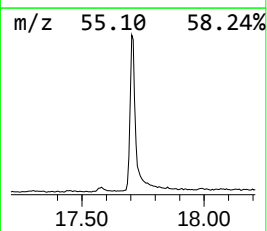
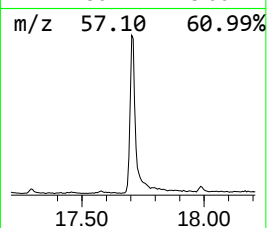
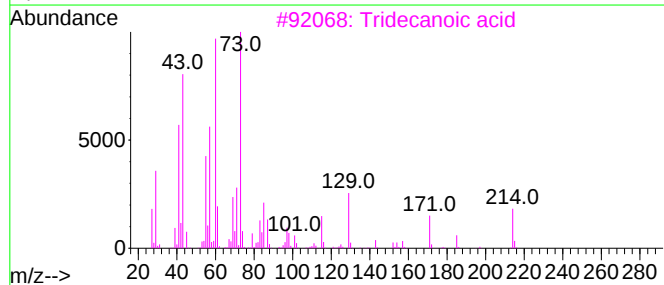
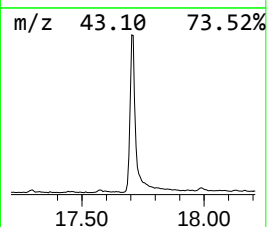
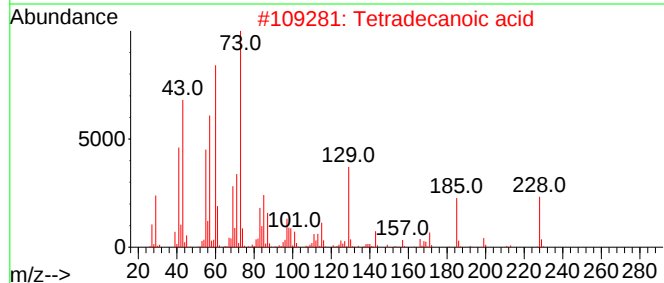
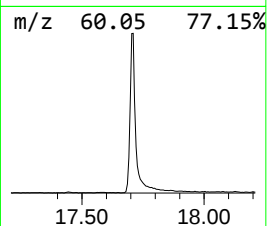
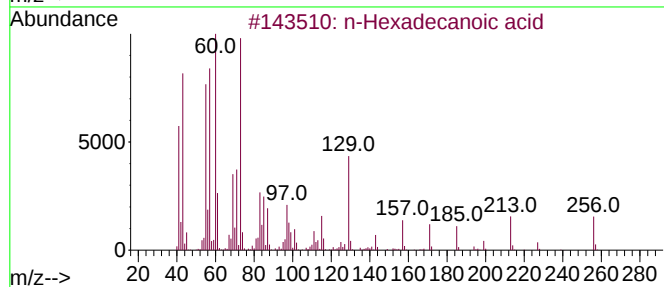
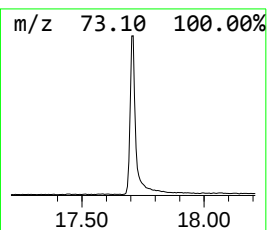
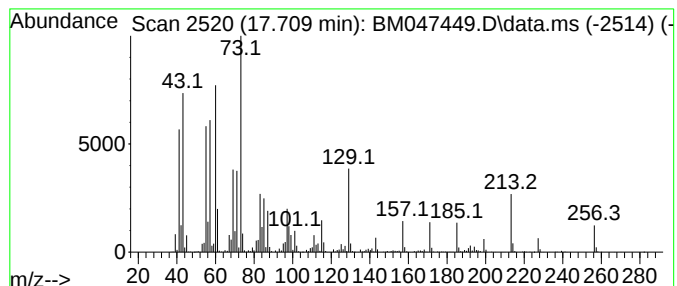
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	20.91 ng	2800230	Phenanthrene-d10	16.774

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	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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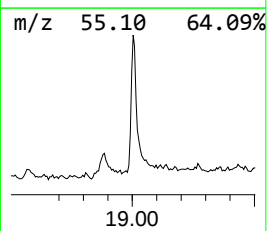
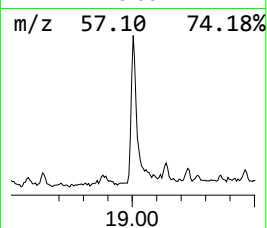
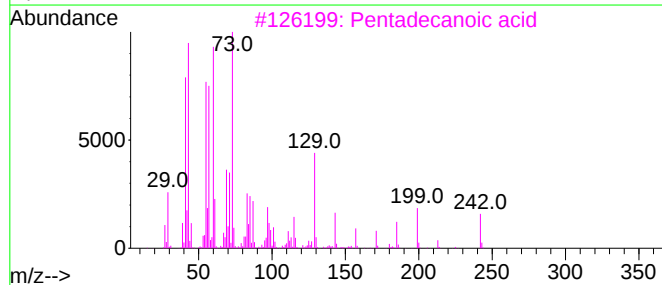
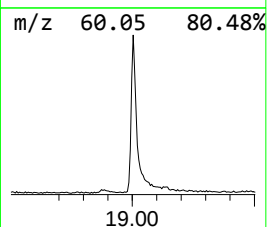
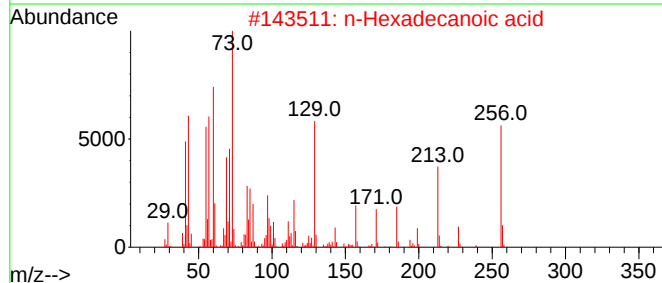
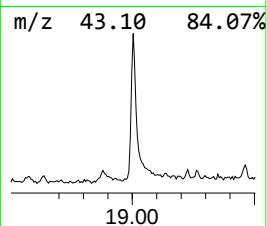
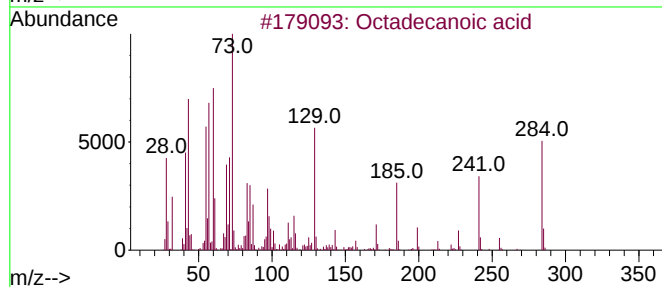
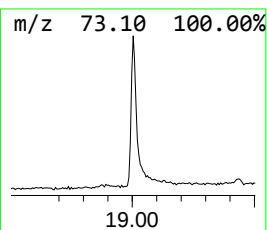
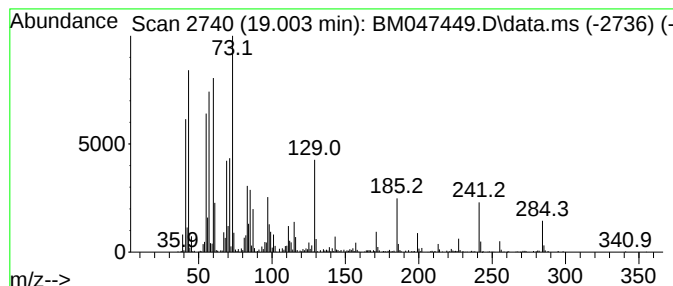
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.003	7.36 ng	900794	Chrysene-d12	21.015

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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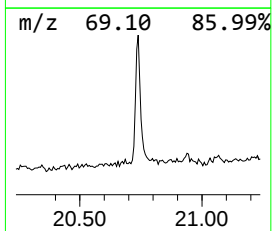
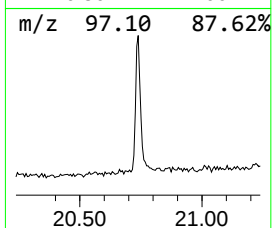
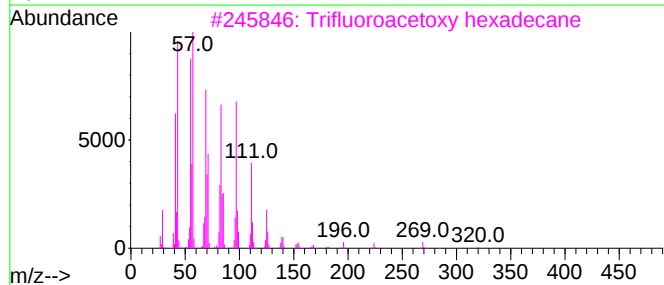
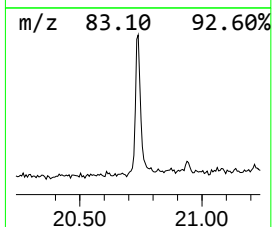
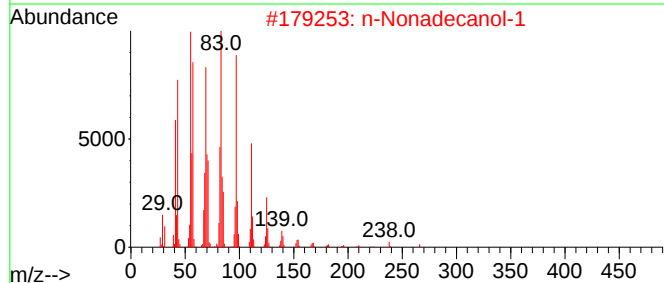
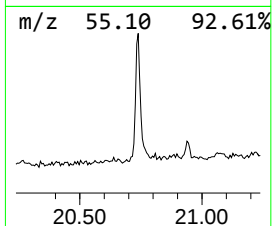
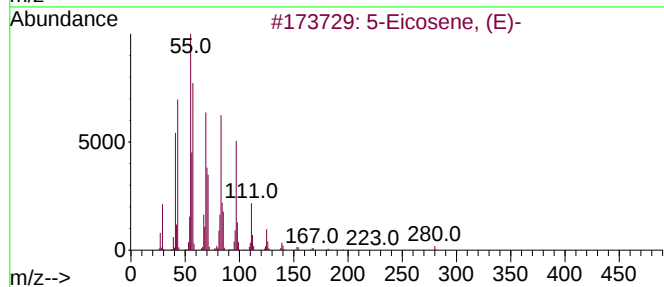
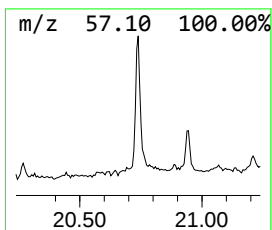
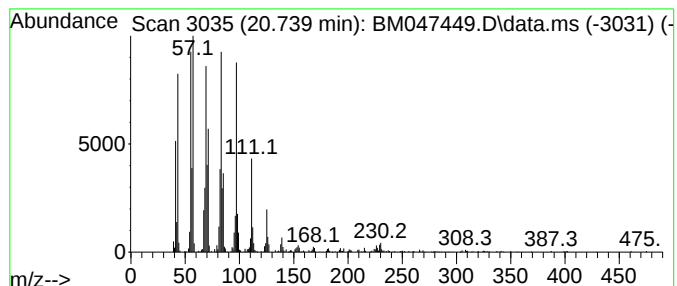
Instrument :
BNA_M
ClientSampleId :
DN-B-38(B-8)

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 7 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.739	4.95 ng	605015	Chrysene-d12		21.015	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	n-Nonadecanol-1		284	C19H40O	001454-84-8	94
3	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
4	Behenic alcohol		326	C22H46O	000661-19-8	94
5	1-Hexacosene		364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090524\
Data File : BM047449.D
Acq On : 05 Sep 2024 16:06
Operator : RC/JU
Sample : P3836-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DN-B-38(B-8)

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	2.0	ng	165235	1	7.339	1624550	20.0
2-Pentanone, 4-...	4.551	7.7	ng	625112	1	7.339	1624550	20.0
Benzophenone	15.392	6.4	ng	860564	4	16.774	2677930	20.0
n-Hexadecanoic ...	17.709	20.9	ng	2800230	4	16.774	2677930	20.0
Octadecanoic acid	19.003	7.4	ng	900794	5	21.015	2446640	20.0
5-Eicosene, (E)-	20.739	5.0	ng	605015	5	21.015	2446640	20.0