

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
 Data File : BM049932.D
 Acq On : 15 Apr 2025 13:17
 Operator : RC/JU
 Sample : Q1781-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-12

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-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049932.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	318	323	332	rBV	295534	420112	2.36%	0.436%
2	5.357	397	403	421	rBV	3817114	5574069	31.29%	5.784%
3	5.963	501	506	515	rVB	187713	282835	1.59%	0.293%
4	6.951	666	674	692	rBV	3336442	5447987	30.59%	5.653%
5	7.769	806	813	821	rBV	1315545	2022808	11.36%	2.099%
6	8.928	1002	1010	1023	rBV	1937662	3321176	18.65%	3.446%
7	10.563	1278	1288	1301	rBV	1494731	2531022	14.21%	2.626%
8	13.033	1701	1708	1726	rBV	6080496	8304825	46.62%	8.618%
9	14.415	1935	1943	1957	rBV	2326514	3438781	19.31%	3.568%
10	15.774	2168	2174	2187	rBV	450661	684548	3.84%	0.710%
11	15.904	2187	2196	2213	rBV	5307733	7589874	42.61%	7.876%
12	17.156	2403	2409	2415	rBV2	2725034	3870638	21.73%	4.017%
13	18.068	2556	2564	2588	rBV	6547105	13246336	74.37%	13.746%
14	19.145	2743	2747	2751	rBV	239849	274764	1.54%	0.285%
15	19.221	2753	2760	2768	rBV2	354377	843654	4.74%	0.875%
16	19.350	2774	2782	2813	rBV	9307162	17812575	100.00%	18.484%
17	19.580	2818	2821	2829	rVB	265673	502443	2.82%	0.521%
18	19.786	2851	2856	2863	rVB	9958829	11343720	63.68%	11.771%
19	21.080	3073	3076	3084	rBV	202902	314374	1.76%	0.326%
20	21.397	3124	3130	3135	rBV	2898381	4138158	23.23%	4.294%
21	24.397	3633	3640	3653	rVB	1705757	4402935	24.72%	4.569%

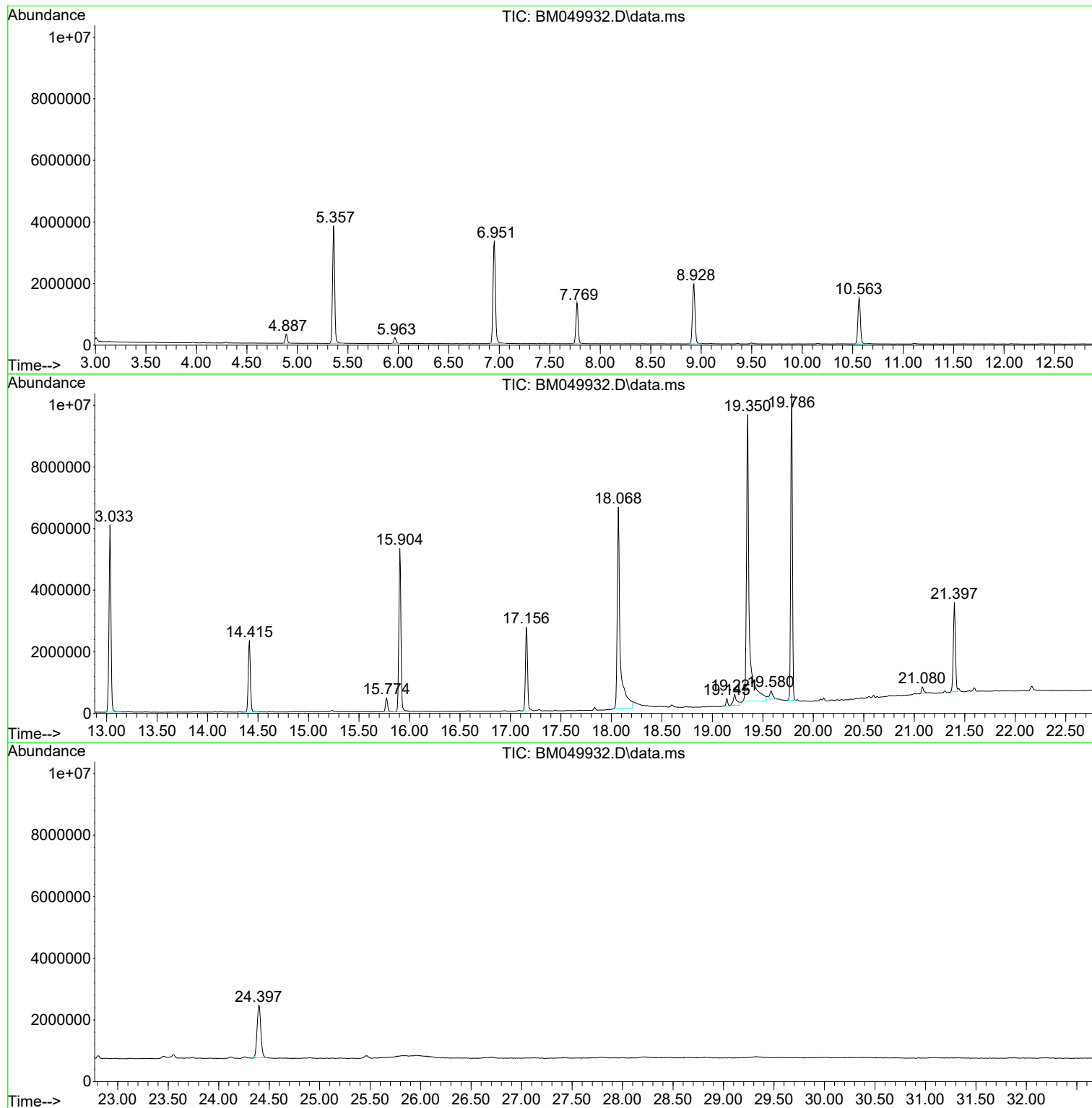
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : RC/JU
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Instrument :
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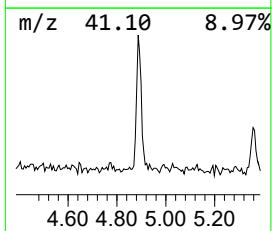
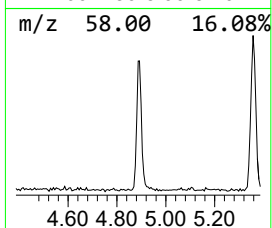
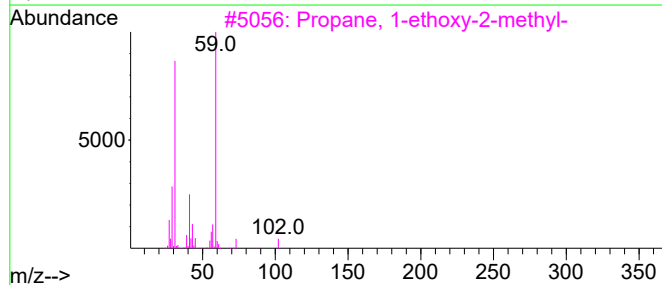
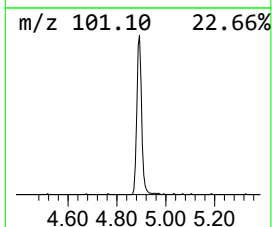
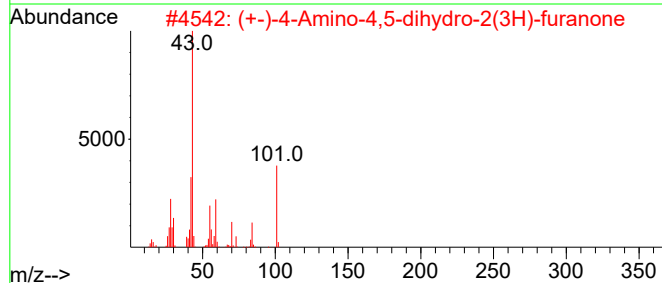
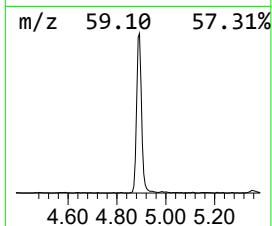
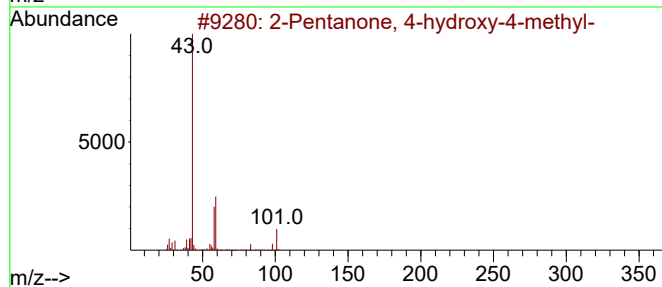
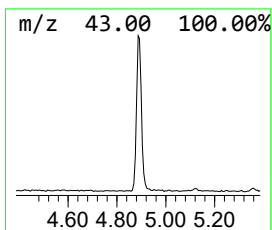
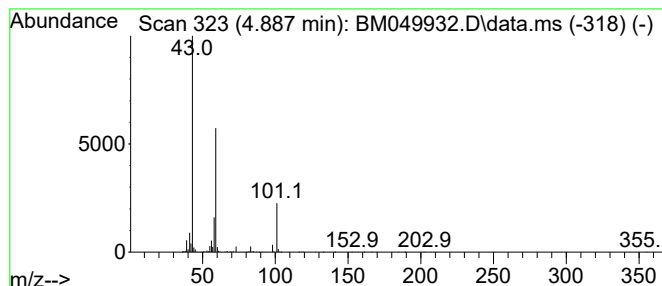
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	4.15 ng	420112	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9



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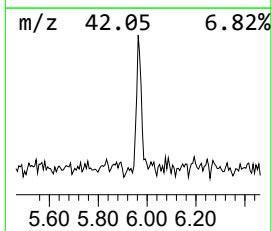
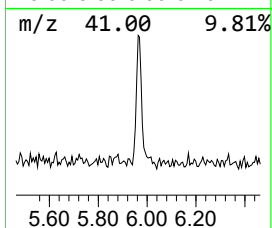
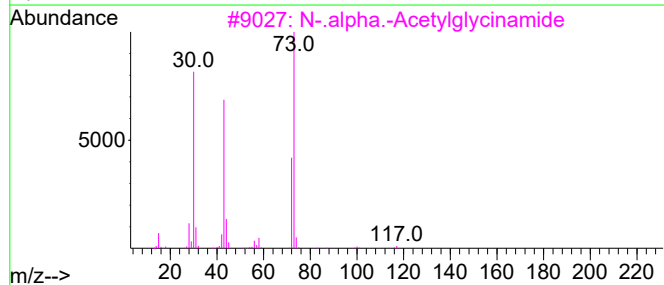
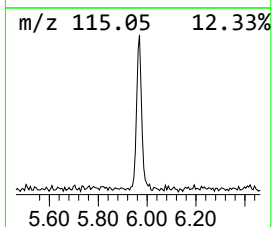
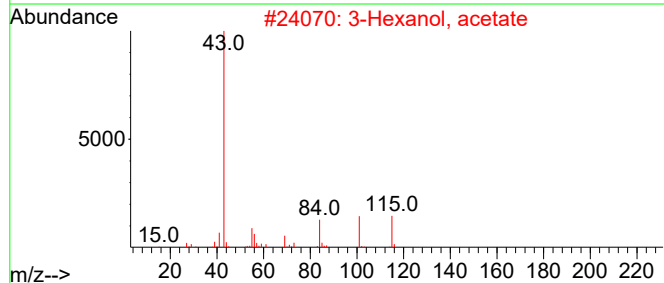
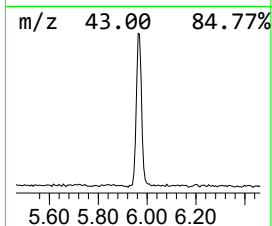
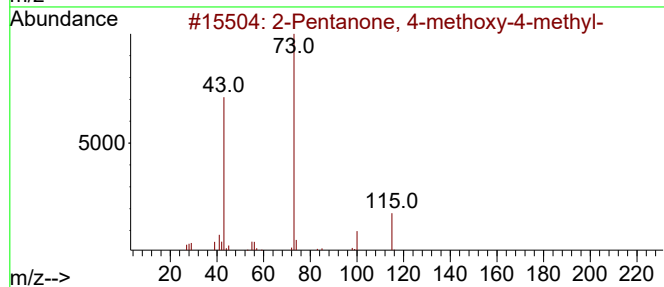
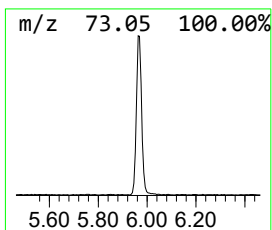
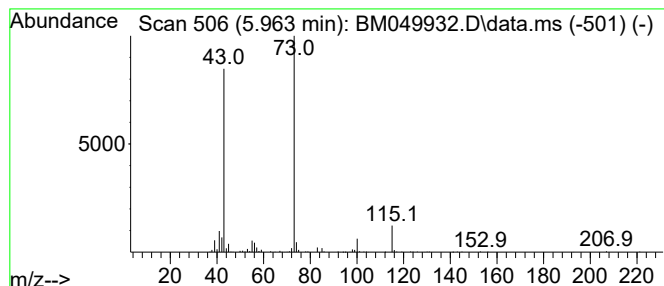
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.963	2.80 ng	282835	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			3-Hexanol, acetate	144	C8H16O2	040780-64-1	32
3			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
5			1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	17



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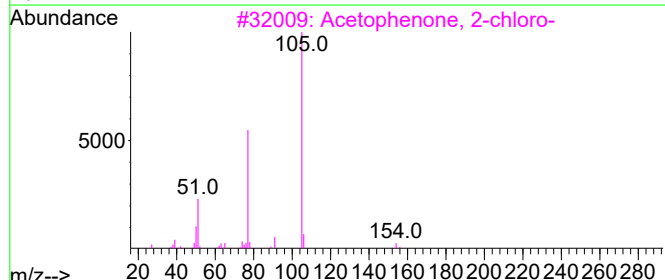
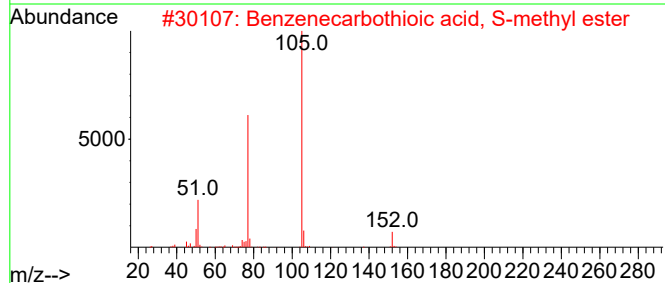
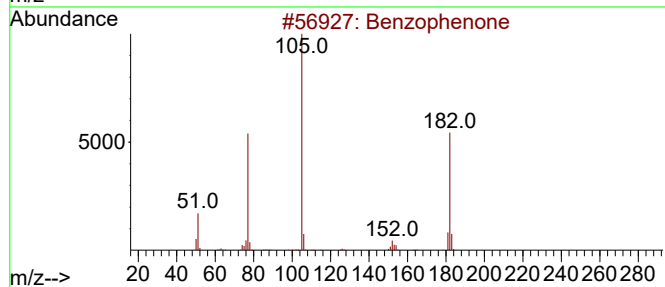
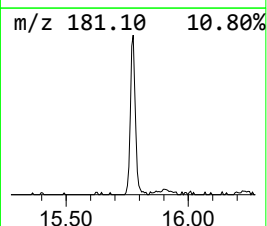
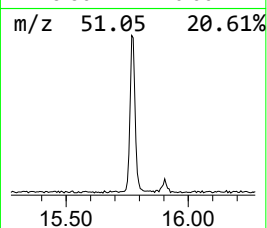
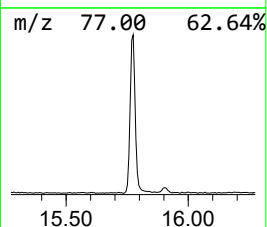
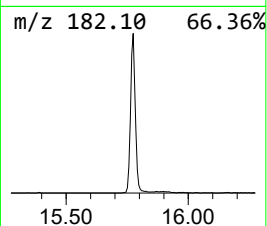
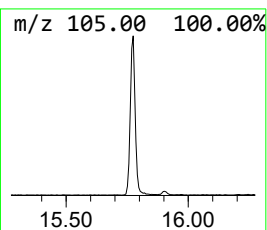
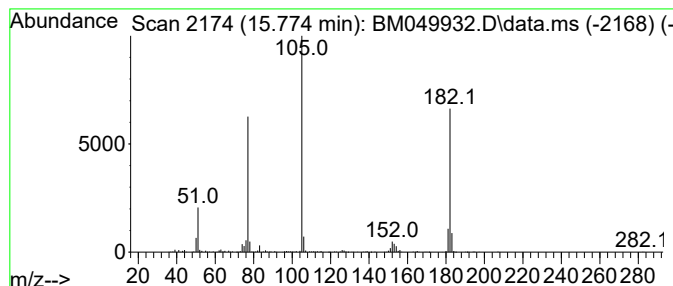
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	3.98 ng	684548	Acenaphthene-d10	14.415

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-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	43
5			Vinyl benzoate	148	C9H8O2	000769-78-8	43



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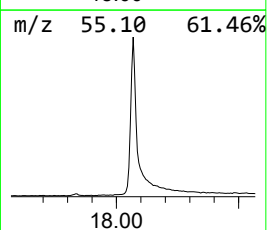
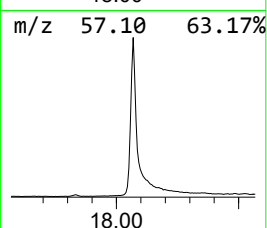
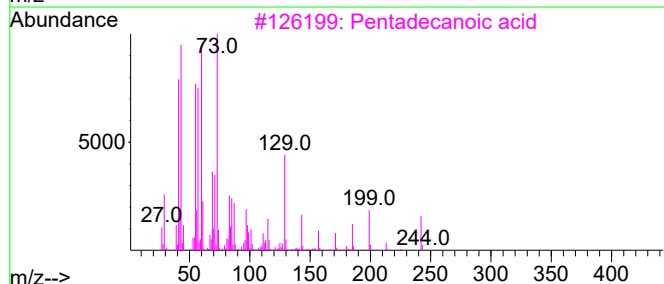
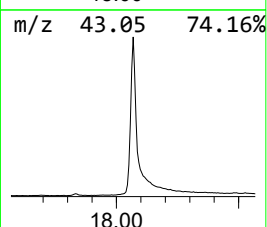
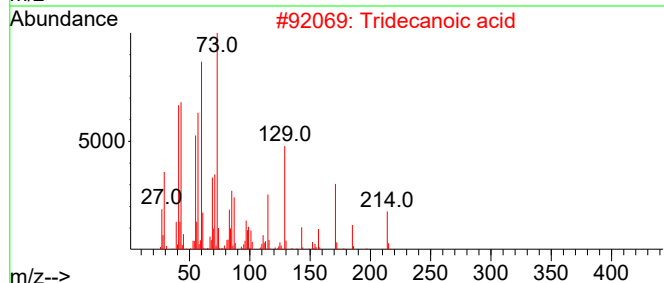
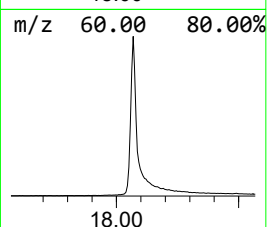
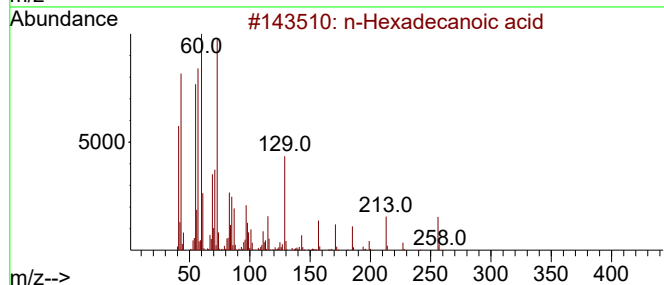
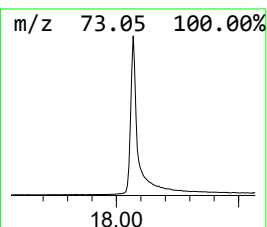
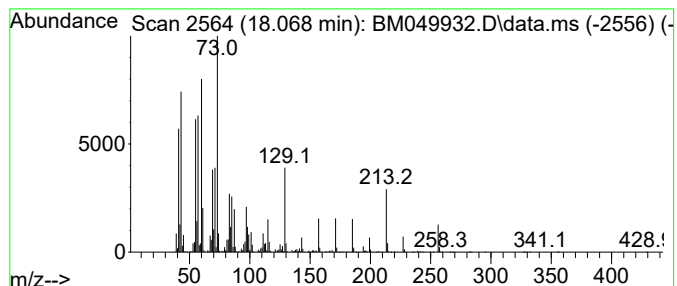
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.068	68.45 ng	13246300	Phenanthrene-d10	17.156

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	68



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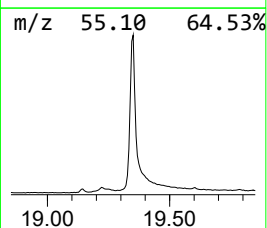
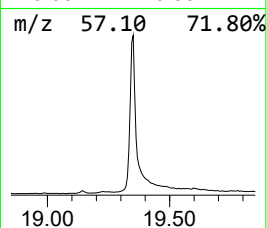
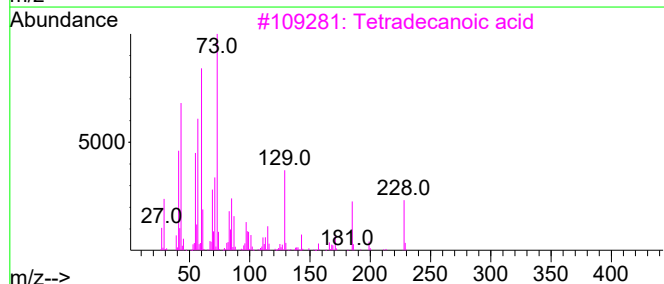
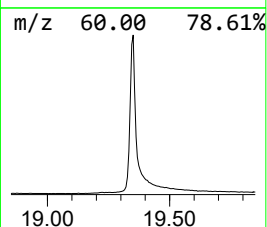
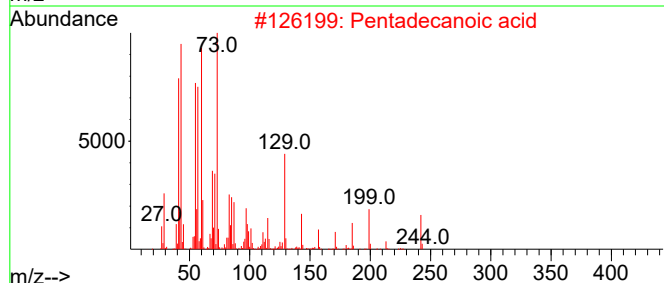
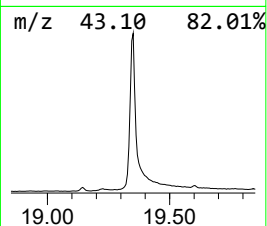
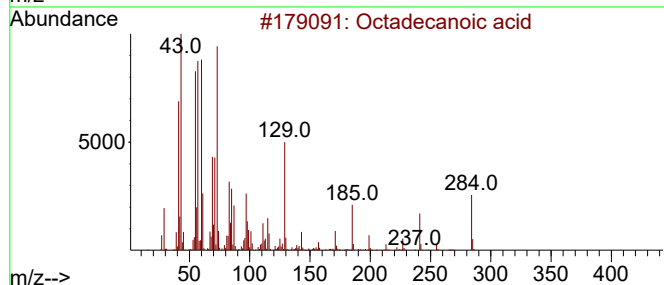
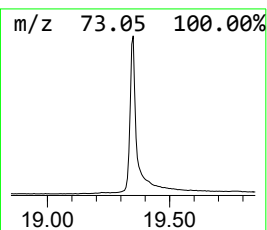
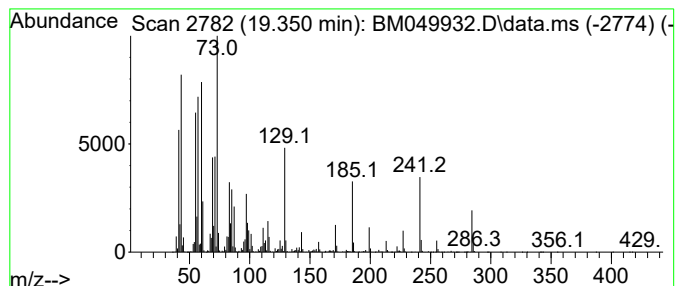
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Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.350	86.09 ng	17812600	Chrysene-d12	21.397

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.887	4.2	ng	420112	1	7.769	2022810	20.0
2-Pentanone, 4-...	5.963	2.8	ng	282835	1	7.769	2022810	20.0
Benzophenone	15.774	4.0	ng	684548	3	14.415	3438780	20.0
n-Hexadecanoic ...	18.068	68.5	ng	13246300	4	17.156	3870640	20.0
Octadecanoic acid	19.350	86.1	ng	17812600	5	21.397	4138160	20.0