

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
 Data File : BM029530.D
 Acq On : 16 Apr 2021 20:11
 Operator : CG/JU
 Sample : M2050-15 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-1

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-BM040121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.922	3	6	27	rVB	498511	668903	37.04%	3.441%
2	5.275	399	406	415	rBV	792624	1174097	65.02%	6.039%
3	6.851	666	674	688	rBV	770398	1282456	71.02%	6.596%
4	7.316	747	753	759	rBV4	8823	19694	1.09%	0.101%
5	7.675	806	814	823	rBV	427833	686417	38.01%	3.531%
6	8.822	1002	1009	1018	rBV	494209	845141	46.80%	4.347%
7	10.451	1278	1286	1293	rBV	530723	903567	50.04%	4.648%
8	12.928	1701	1707	1720	rVB	940958	1410329	78.11%	7.254%
9	13.216	1749	1756	1762	rBV	83032	130547	7.23%	0.671%
10	13.769	1844	1850	1859	rVB	69975	109361	6.06%	0.563%
11	14.033	1889	1895	1902	rBV2	43411	75129	4.16%	0.386%
12	14.151	1909	1915	1923	rBV3	11000	28071	1.55%	0.144%
13	14.310	1935	1942	1949	rBV	720879	1079010	59.76%	5.550%
14	15.798	2189	2195	2204	rBV	782450	1130656	62.62%	5.816%
15	16.039	2231	2236	2243	rBV8	15189	29954	1.66%	0.154%
16	16.204	2255	2264	2270	rBV9	6944	18809	1.04%	0.097%
17	17.057	2402	2409	2413	rBV	847093	1180280	65.37%	6.071%
18	17.098	2413	2416	2421	rVB	125456	161711	8.96%	0.832%
19	17.186	2427	2431	2436	rVB	53066	75567	4.18%	0.389%
20	17.245	2437	2441	2447	rVB7	11100	20394	1.13%	0.105%
21	17.957	2553	2562	2573	rBV2	180257	405558	22.46%	2.086%
22	18.115	2586	2589	2594	rBV2	36240	60816	3.37%	0.313%
23	18.251	2610	2612	2619	rVB7	12873	19562	1.08%	0.101%
24	18.433	2640	2643	2646	rVB	21236	23856	1.32%	0.123%
25	18.733	2690	2694	2696	rBV3	14284	20744	1.15%	0.107%
26	18.857	2710	2715	2718	rBV2	31351	57198	3.17%	0.294%
27	18.898	2719	2722	2728	rVV7	19533	42854	2.37%	0.220%
28	19.115	2754	2759	2764	rBV	427743	573112	31.74%	2.948%
29	19.245	2777	2781	2788	rBV4	70135	164450	9.11%	0.846%
30	19.474	2812	2820	2829	rVB	420361	671490	37.19%	3.454%
31	19.686	2851	2856	2860	rVB	1303389	1581286	87.57%	8.133%
32	20.068	2919	2921	2925	rVB	48162	58023	3.21%	0.298%
33	20.956	3068	3072	3078	rBV2	263297	331600	18.36%	1.706%
34	21.233	3113	3119	3123	rBV3	1159740	1805668	100.00%	9.288%
35	21.268	3123	3125	3132	rVB	283551	325162	18.01%	1.672%
36	22.780	3378	3382	3387	rBV	275618	542632	30.05%	2.791%

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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-BM040121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.345	3474	3478	3488	rVB	291450	513994	28.47%	2.644%
38	23.445	3489	3495	3500	rBV2	668266	1213649	67.21%	6.242%

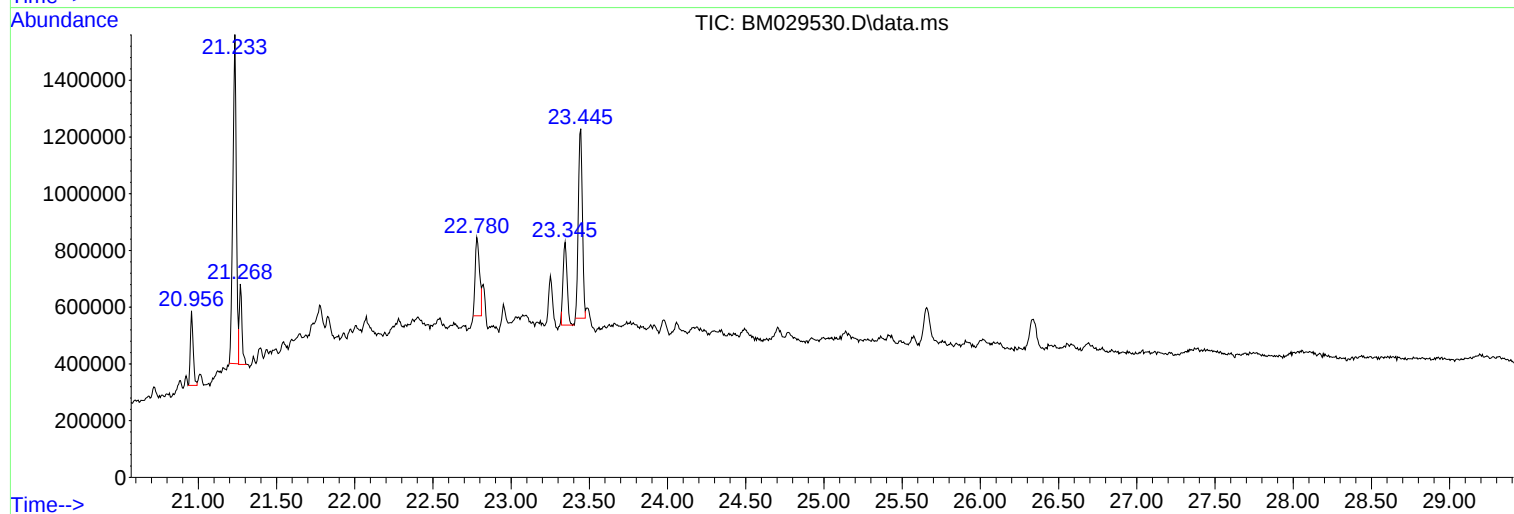
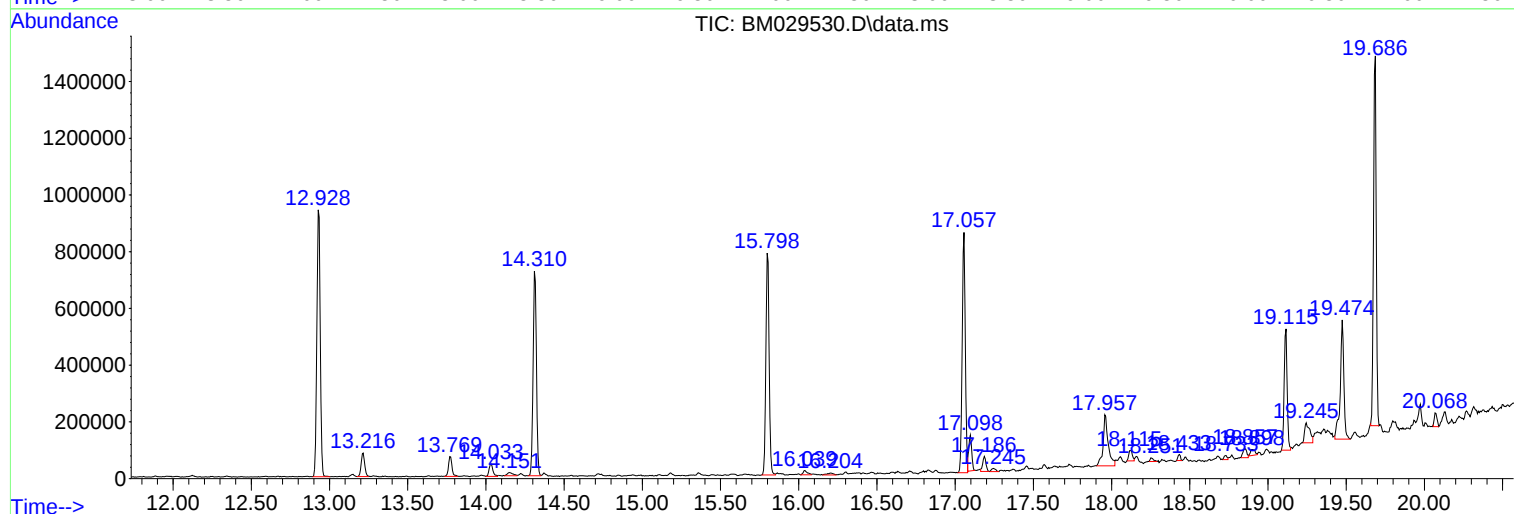
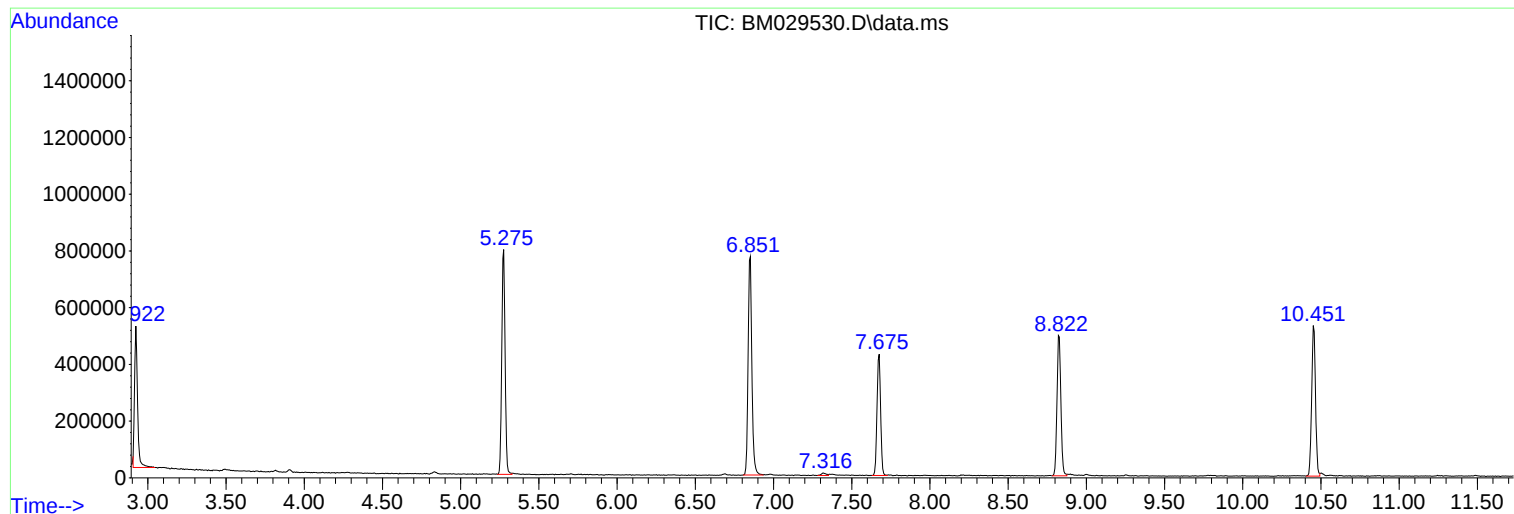
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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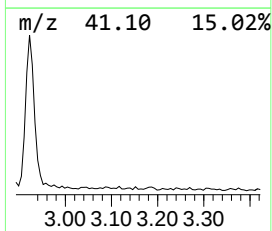
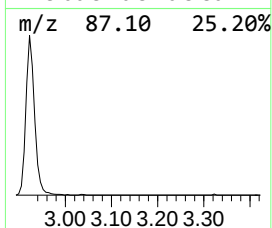
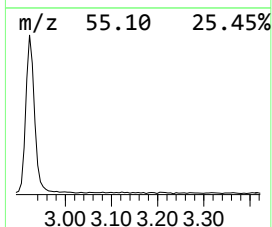
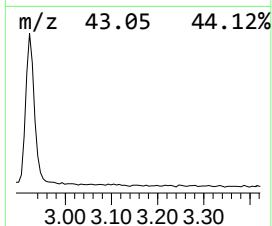
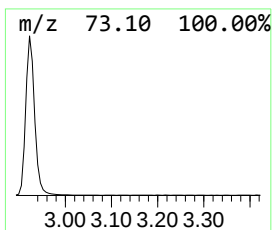
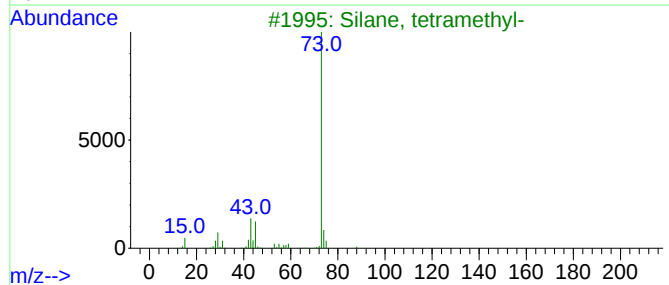
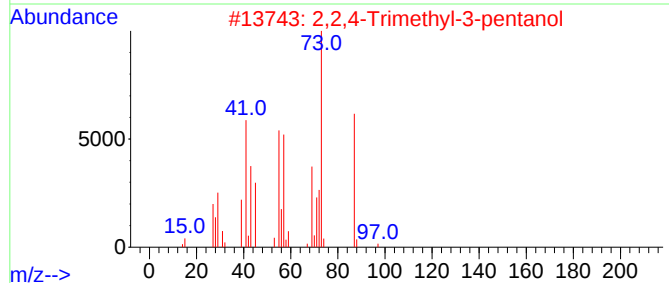
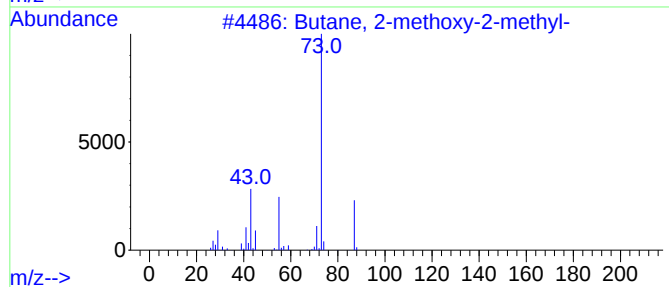
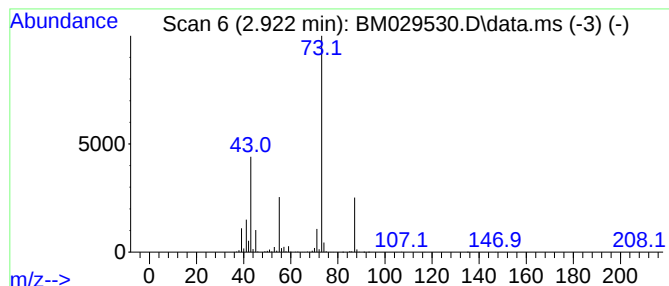
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.922	19.49 ng	668903	1,4-Dichlorobenzene-d4	7.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12



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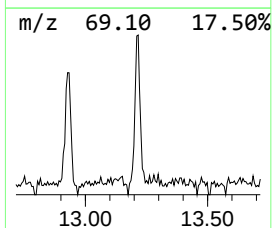
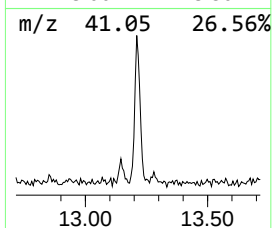
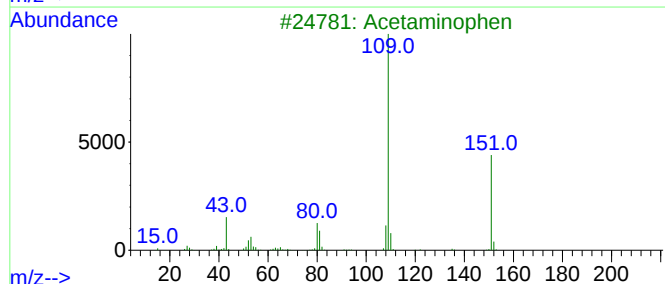
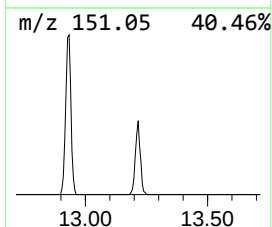
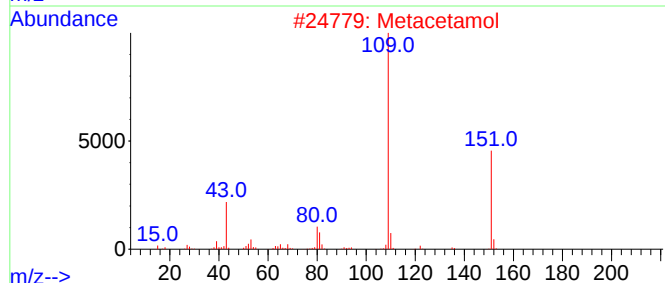
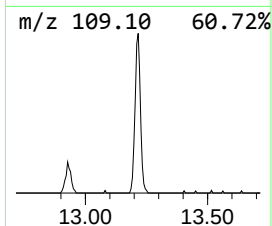
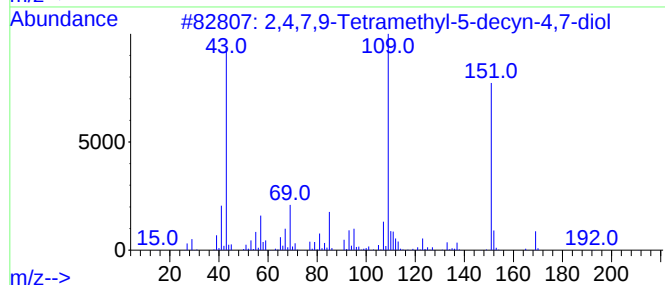
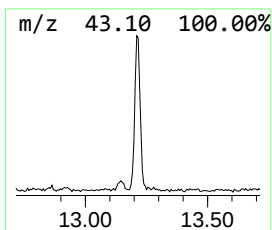
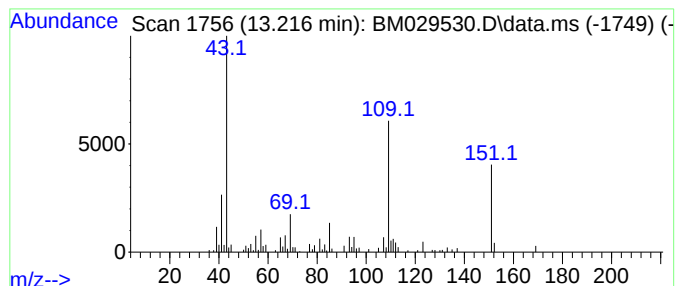
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	2.42 ng	130547	Acenaphthene-d10	14.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Metacetamol	151	C8H9NO2	000621-42-1	58	
3	Acetaminophen	151	C8H9NO2	000103-90-2	53	
4	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	53	
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53	



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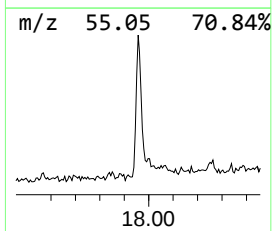
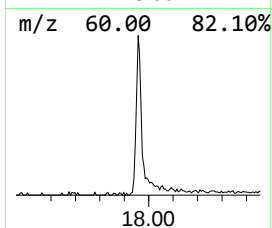
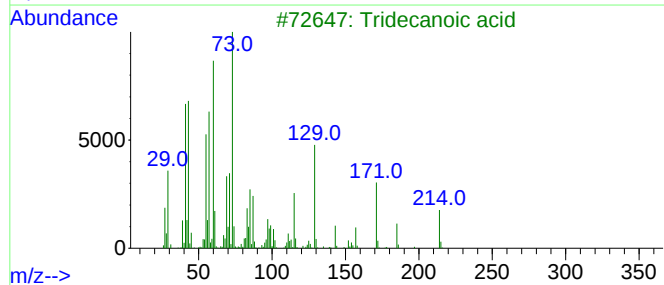
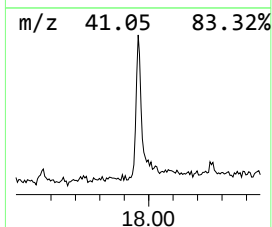
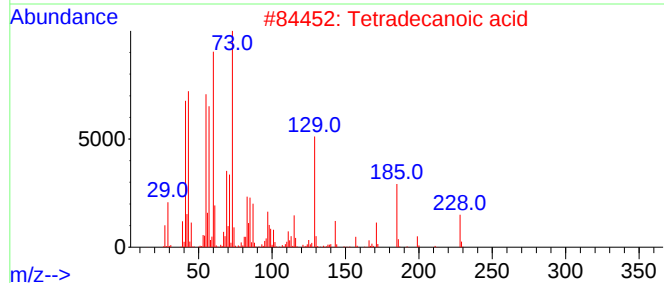
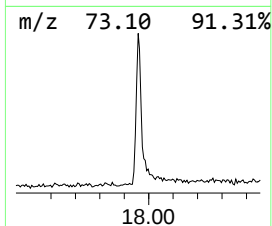
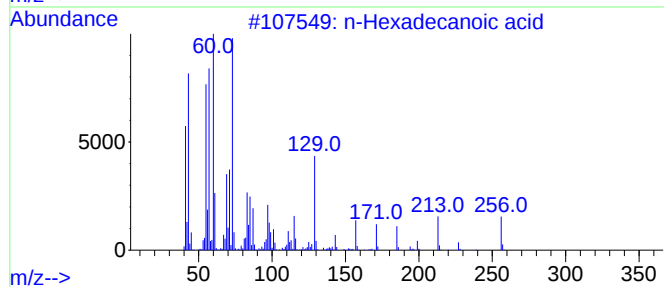
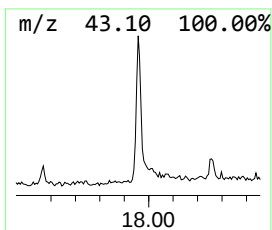
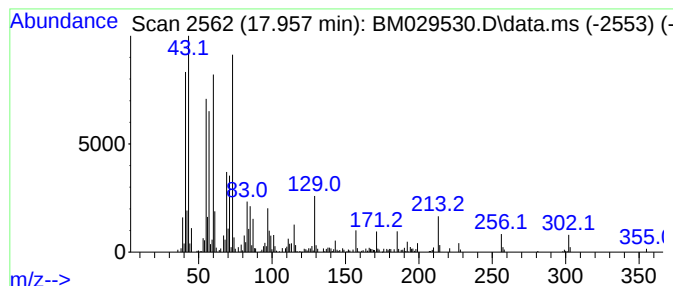
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.957	6.87 ng	405558	Phenanthrene-d10	17.057

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	96
3			Tridecanoic acid	214	C13H26O2	000638-53-9	95
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	72



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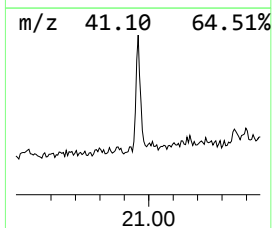
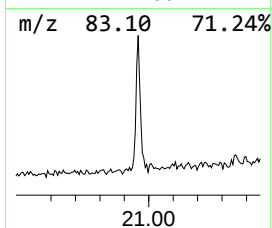
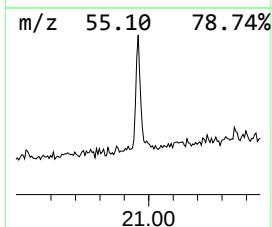
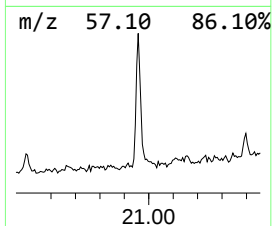
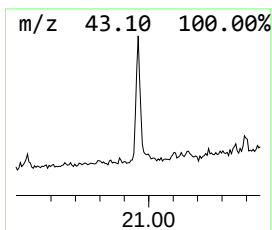
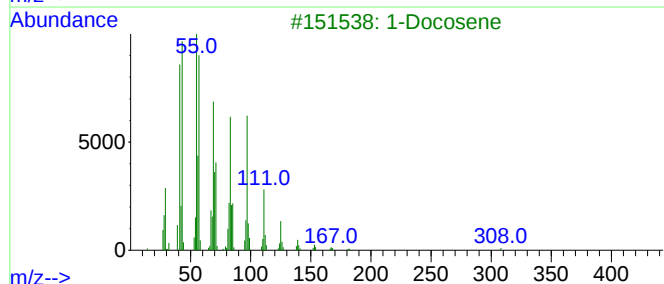
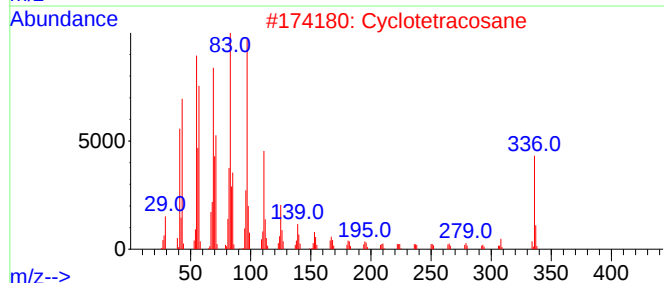
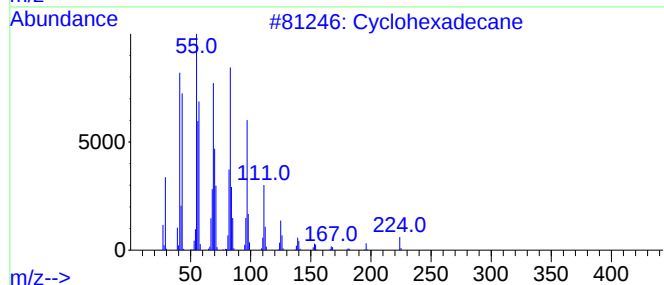
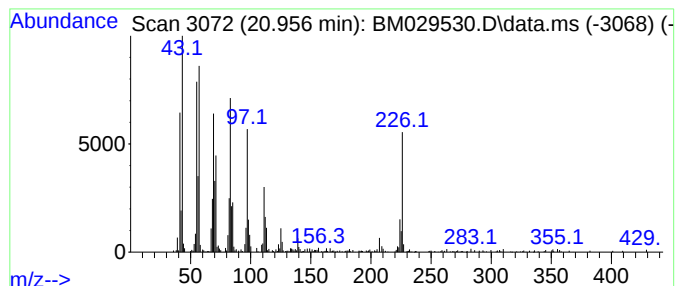
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.956	3.67 ng	331600	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	95
2			Cyclotetracosane	336	C24H48	000297-03-0	93
3			1-Docosene	308	C22H44	001599-67-3	93
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	89
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	89



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.922	19.5	ng	668903	1	7.675	686417	20.0
2,4,7,9-Tetrame...	13.216	2.4	ng	130547	3	14.310	1079010	20.0
n-Hexadecanoic ...	17.957	6.9	ng	405558	4	17.057	1180280	20.0
Cyclohexadecane	20.956	3.7	ng	331600	5	21.233	1805670	20.0