

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030822\
 Data File : BP009304.D
 Acq On : 08 Mar 2022 14:54
 Operator : CG/JU
 Sample : N1730-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 21-22-SAMPLE-LOCATION-11

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_P\Methods\8270E-BP030522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009304.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.070	10	14	27	rVB	796970	1145741	9.41%	1.425%
2	5.411	405	412	429	rVB	4561119	7230376	59.40%	8.994%
3	6.987	671	680	690	rBV	4370881	7463104	61.32%	9.283%
4	7.816	813	821	829	rBV	1428066	2429586	19.96%	3.022%
5	8.969	1008	1017	1027	rBV	2716914	4699106	38.61%	5.845%
6	10.399	1254	1260	1266	rBV	87374	154847	1.27%	0.193%
7	10.610	1286	1296	1305	rBV	1785545	3184801	26.17%	3.962%
8	13.081	1708	1716	1729	rBV	6044829	9672944	79.47%	12.032%
9	14.116	1887	1892	1900	rVB3	87433	150247	1.23%	0.187%
10	14.457	1943	1950	1960	rBV	2357710	3786925	31.11%	4.710%
11	15.281	2085	2090	2094	rBV2	95536	143856	1.18%	0.179%
12	15.622	2142	2148	2159	rVB	72770	169550	1.39%	0.211%
13	15.945	2197	2203	2213	rBV	4330056	6772537	55.64%	8.424%
14	16.604	2309	2315	2324	rVB5	100160	235566	1.94%	0.293%
15	17.157	2405	2409	2413	rBV2	122301	168224	1.38%	0.209%
16	17.216	2413	2419	2431	rVB	2750150	4355337	35.78%	5.418%
17	17.516	2466	2470	2475	rBV	74009	131797	1.08%	0.164%
18	17.910	2533	2537	2541	rVB2	91251	126162	1.04%	0.157%
19	18.122	2568	2573	2579	rBV	290261	440824	3.62%	0.548%
20	18.187	2580	2584	2589	rVB	168872	224686	1.85%	0.279%
21	18.381	2612	2617	2620	rBV	216675	330142	2.71%	0.411%
22	18.422	2620	2624	2641	rVB2	419052	797898	6.56%	0.992%
23	19.239	2757	2763	2773	rVB4	134782	300169	2.47%	0.373%
24	19.363	2780	2784	2787	rBV3	148148	210102	1.73%	0.261%
25	19.592	2819	2823	2830	rBV3	104723	220732	1.81%	0.275%
26	19.792	2851	2857	2869	rVB	9110656	12171648	100.00%	15.140%
27	21.045	3066	3070	3074	rBV2	455178	691530	5.68%	0.860%
28	21.104	3075	3080	3090	rVB2	529820	1247731	10.25%	1.552%
29	21.322	3111	3117	3131	rBV	3867524	5457124	44.83%	6.788%
30	23.722	3519	3525	3543	rVB2	2780727	6280454	51.60%	7.812%

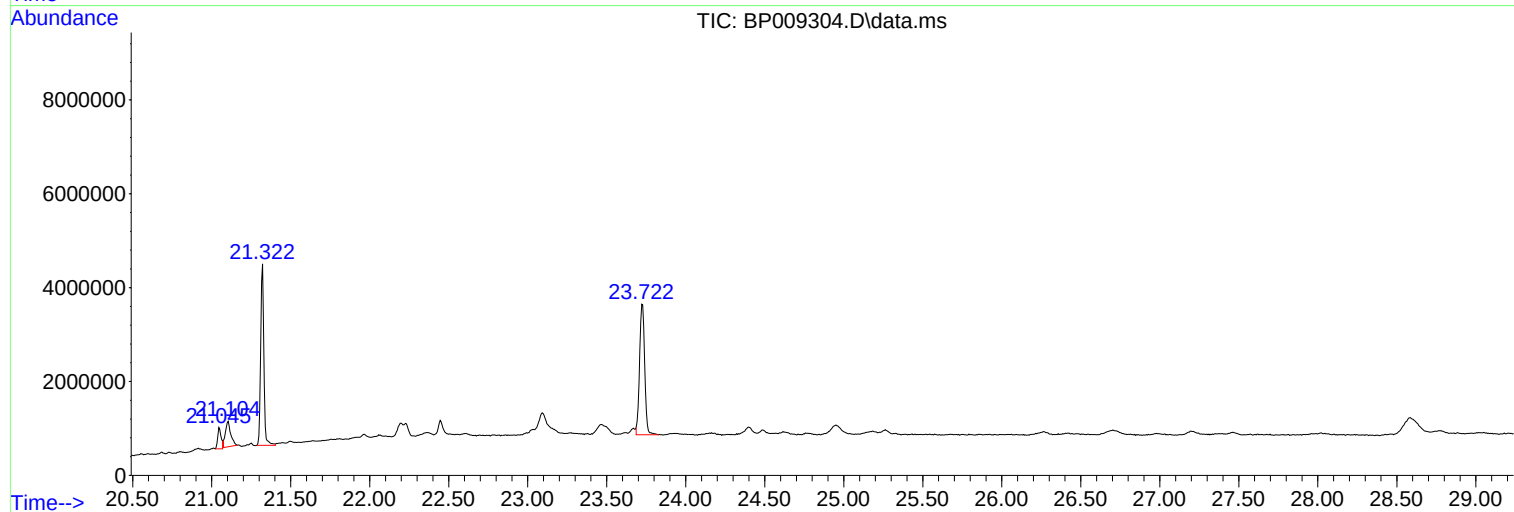
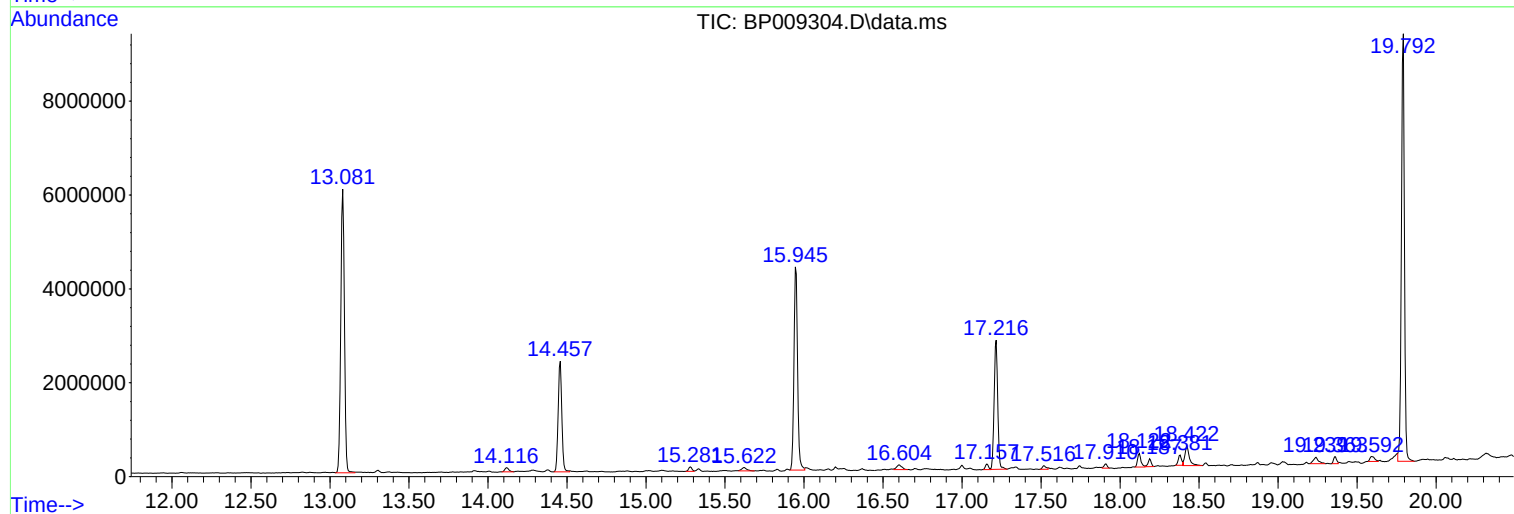
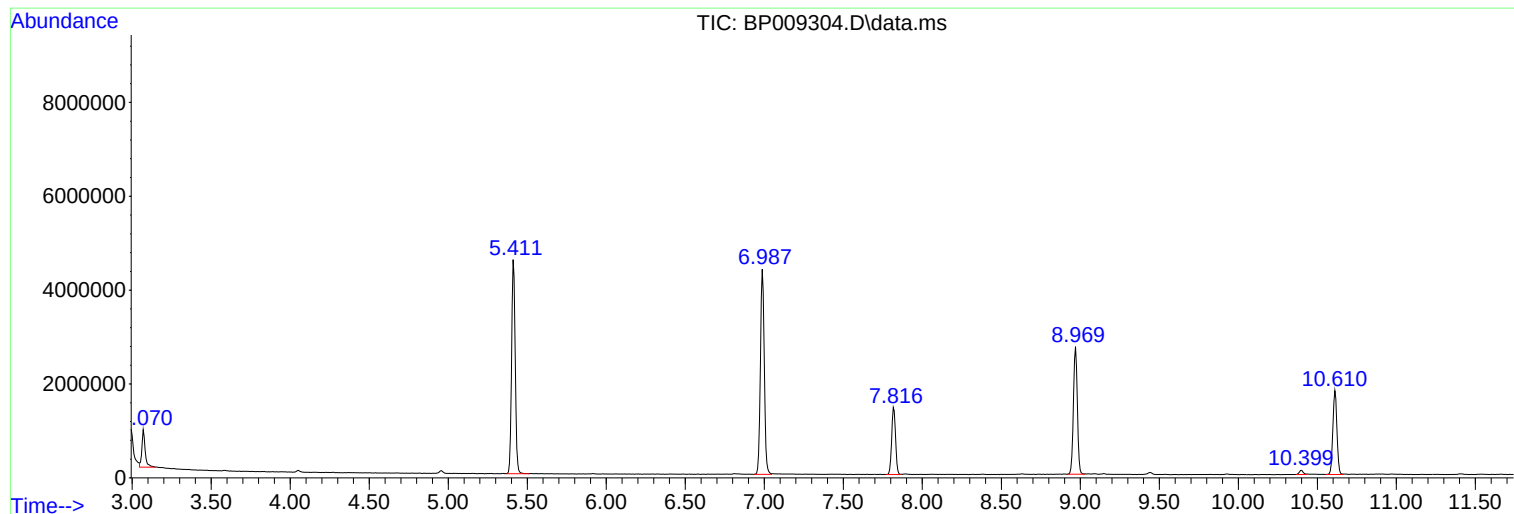
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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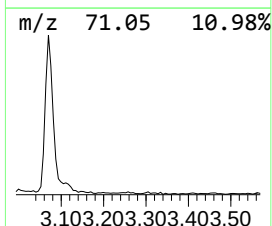
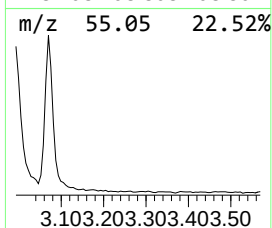
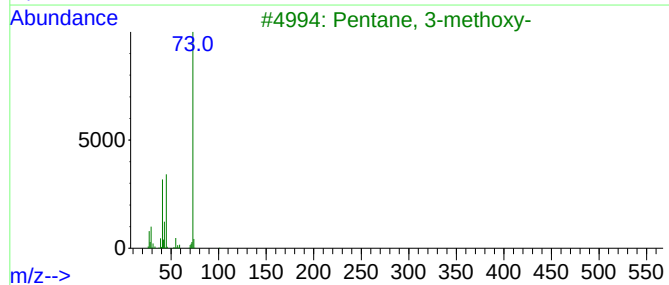
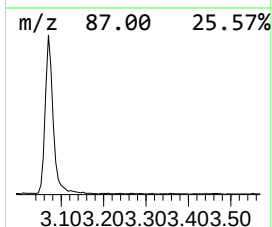
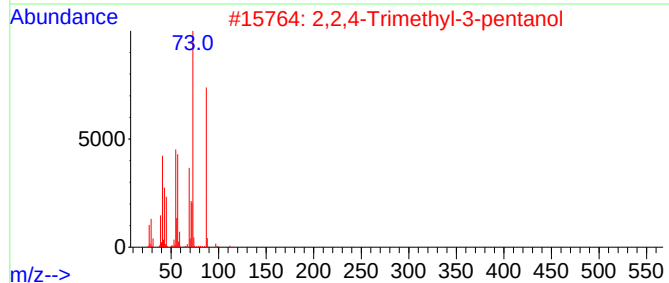
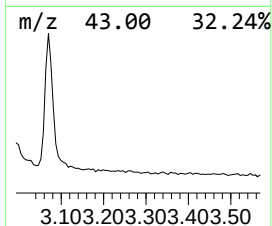
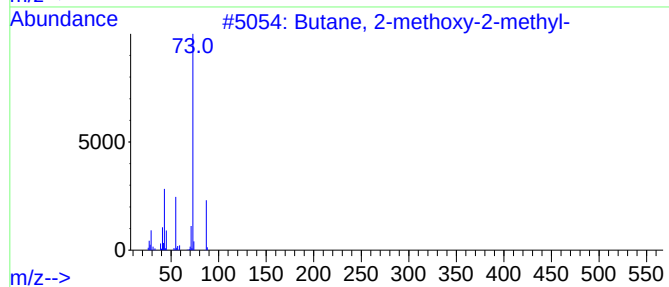
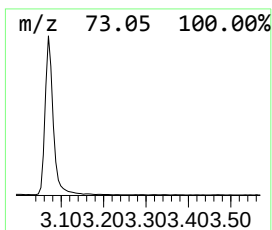
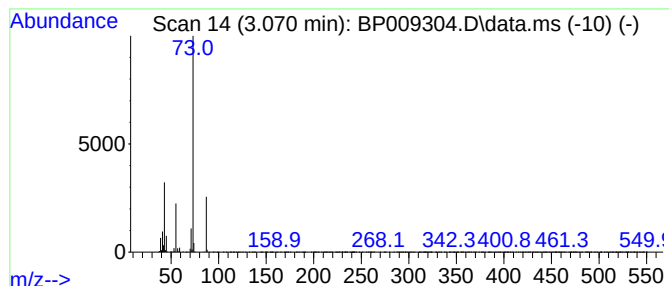
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
3.070	9.43 ng	1145740	1,4-Dichlorobenzene-d4	7.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16



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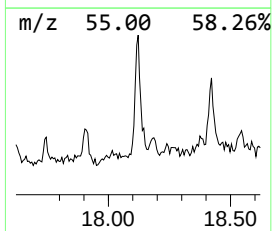
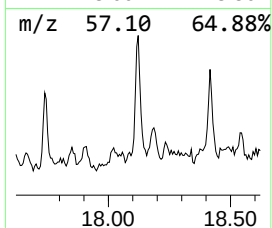
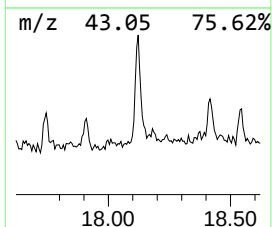
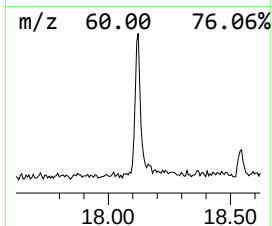
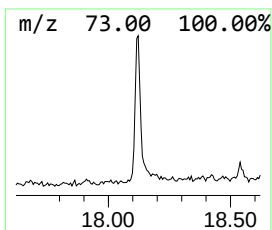
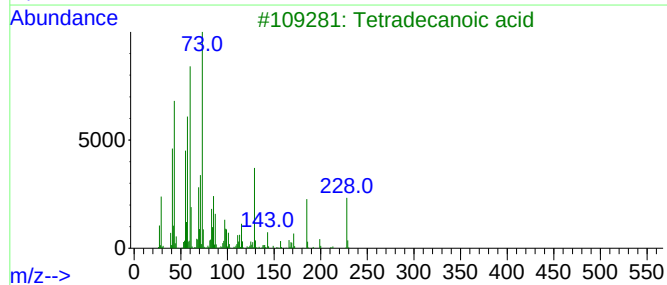
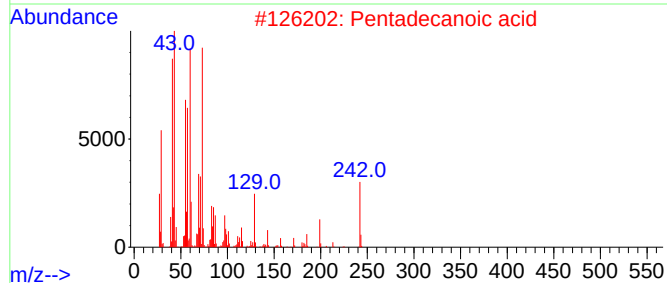
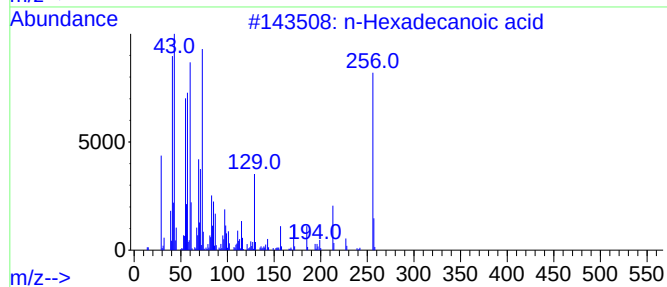
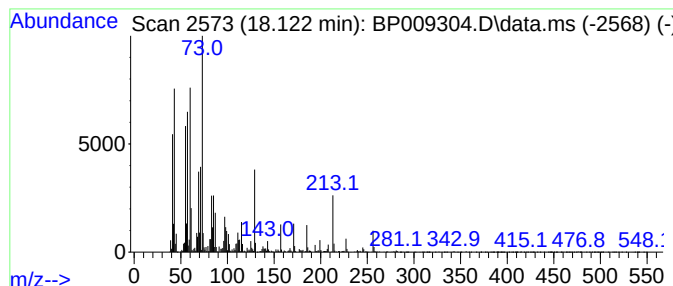
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.122	2.02 ng	440824	Phenanthrene-d10	17.216

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	91
5		Octadecanoic acid	284	C18H36O2	000057-11-4	81



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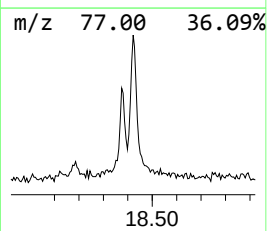
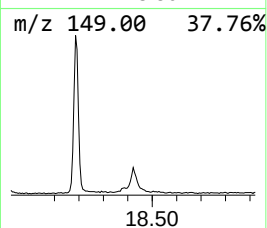
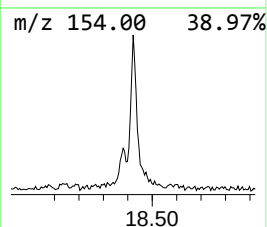
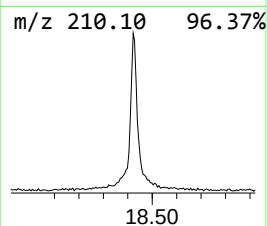
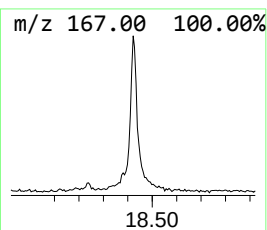
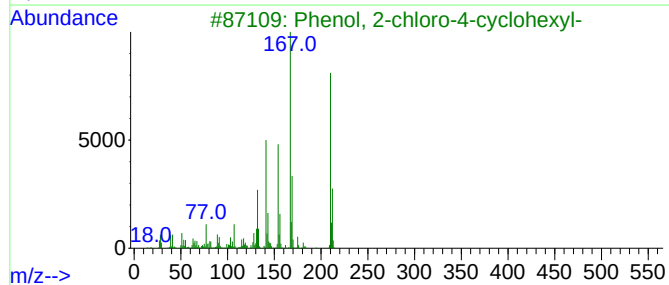
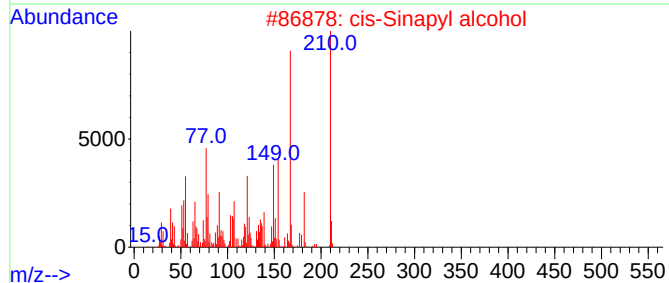
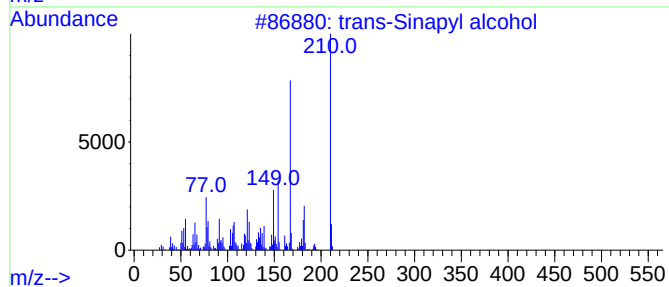
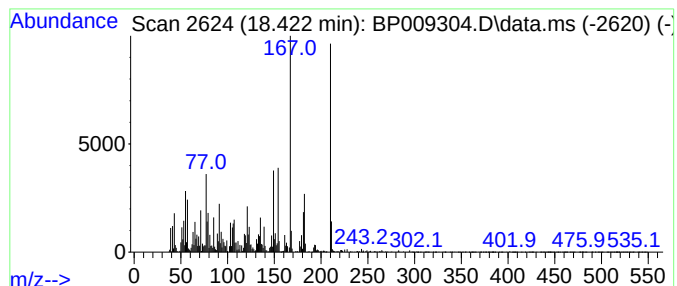
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 trans-Sinapyl alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.422	3.66 ng	797898	Phenanthrene-d10	17.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	95
2			cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	93
3			Phenol, 2-chloro-4-cyclohexyl-	210	C12H15ClO	003964-61-2	64
4			2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	60
5			Syringylacetone	210	C11H14O4	019037-58-2	60



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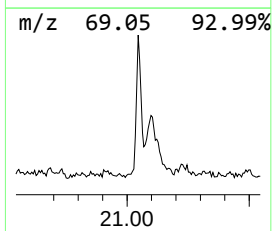
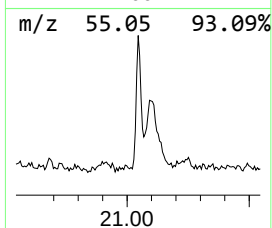
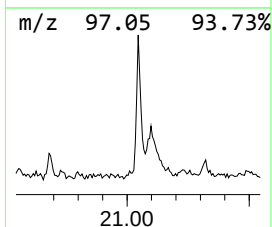
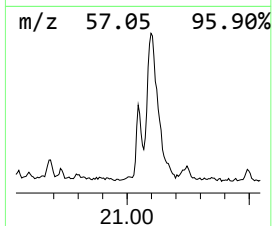
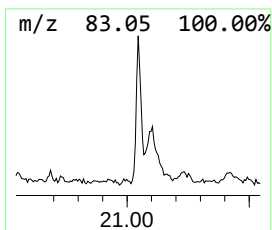
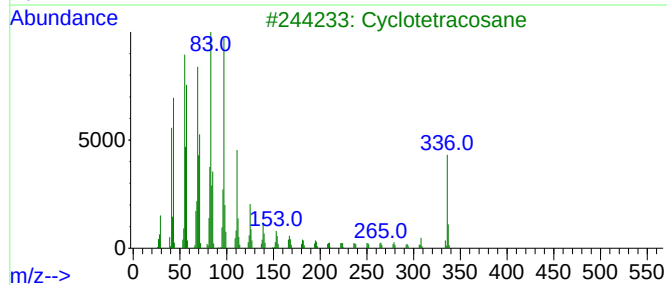
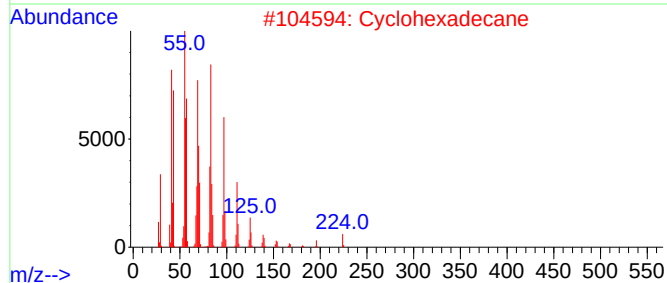
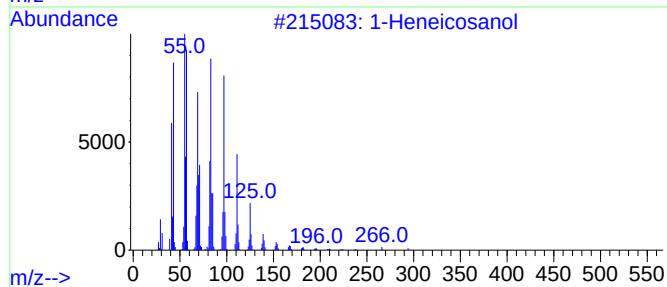
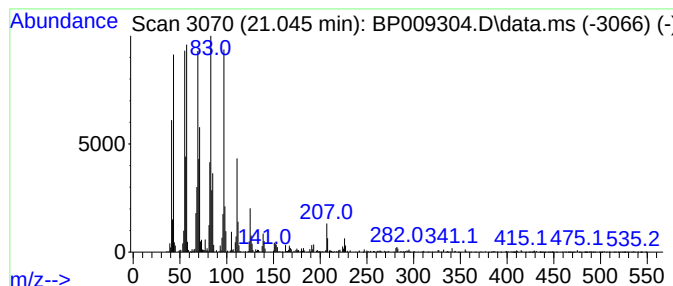
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.045	2.53 ng	691530	Chrysene-d12	21.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Cyclohexadecane	224	C16H32	000295-65-8	95
3			Cyclotetracosane	336	C24H48	000297-03-0	94
4			1-Tetracosene	336	C24H48	010192-32-2	94
5			Pentacos-1-ene	350	C25H50	016980-85-1	94



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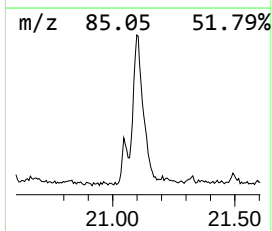
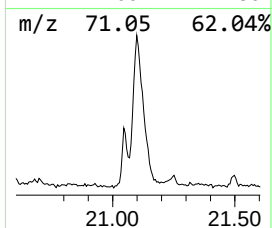
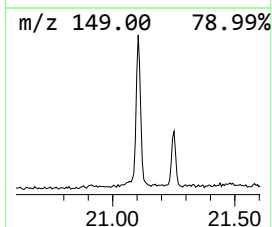
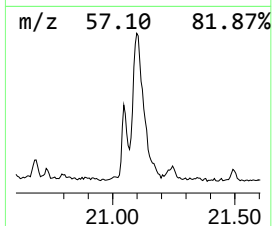
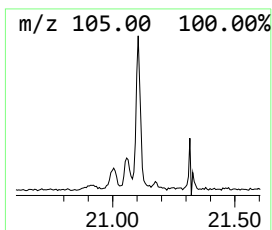
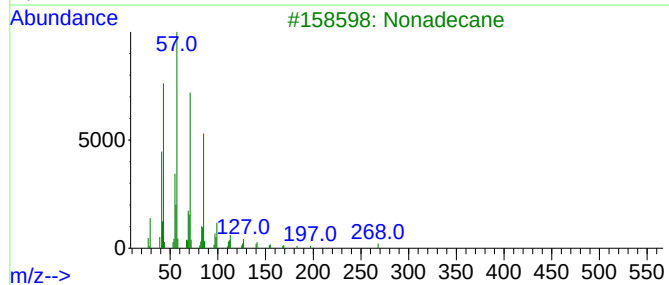
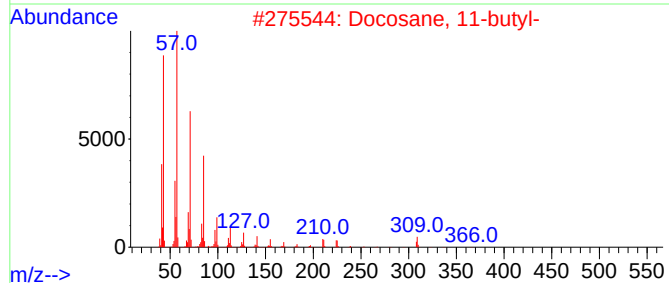
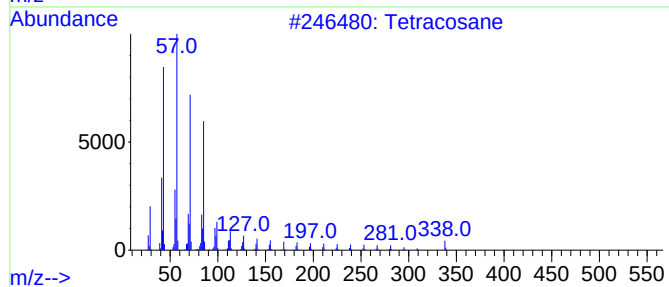
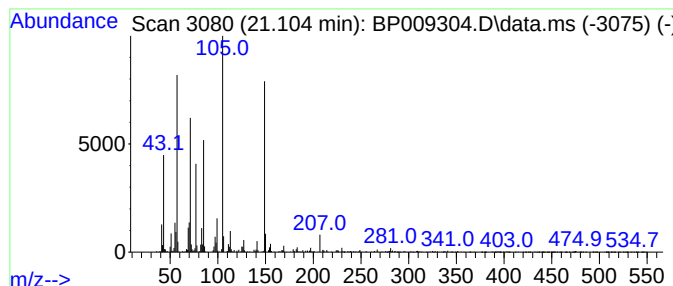
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	4.57 ng	1247730	Chrysene-d12	21.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	58
2			Docosane, 11-butyl-	366	C26H54	013475-76-8	47
3			Nonadecane	268	C19H40	000629-92-5	46
4			Hexatriacontane	507	C36H74	000630-06-8	38
5			Heptadecane	240	C17H36	000629-78-7	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.070	9.4	ng	1145740	1	7.816	2429590	20.0
n-Hexadecanoic ...	18.122	2.0	ng	440824	4	17.216	4355340	20.0
trans-Sinapyl a...	18.422	3.7	ng	797898	4	17.216	4355340	20.0
1-Heneicosanol	21.045	2.5	ng	691530	5	21.322	5457120	20.0
Tetracosane	21.104	4.6	ng	1247730	5	21.322	5457120	20.0