

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032122\
 Data File : BM034286.D
 Acq On : 21 Mar 2022 12:35
 Operator : CG/JU
 Sample : N1870-06
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PT-ACIDS-WP

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-BM031522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034286.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.496	377	384	398	rBV	3678533	5252898	41.65%	4.015%
2	7.107	649	658	660	rBV	3338720	6083336	48.24%	4.649%
3	7.131	660	662	681	rVB	3543959	4587538	36.38%	3.506%
4	7.501	718	725	735	rBV	901753	1409167	11.17%	1.077%
5	7.943	793	800	809	rVB	690283	1058176	8.39%	0.809%
6	8.707	923	930	946	rBV	2045301	3252310	25.79%	2.486%
7	9.107	989	998	1006	rBV	2270907	3667671	29.08%	2.803%
8	9.866	1119	1127	1132	rBV	2891647	4774759	37.86%	3.649%
9	9.925	1132	1137	1153	rVB	3067257	4882081	38.71%	3.731%
10	10.401	1210	1218	1235	rBV	4154608	6655069	52.77%	5.086%
11	10.754	1269	1278	1291	rVB	885999	1481346	11.75%	1.132%
12	10.937	1300	1309	1321	rBV	4309553	7044383	55.86%	5.384%
13	12.036	1486	1496	1512	rBV	5893214	9180319	72.79%	7.016%
14	13.019	1656	1663	1669	rBV	3092269	4921405	39.02%	3.761%
15	13.089	1669	1675	1689	rVV	6757113	10265373	81.40%	7.846%
16	13.213	1689	1696	1712	rVB	5851047	8595204	68.15%	6.569%
17	13.889	1805	1811	1820	rBV	129073	202913	1.61%	0.155%
18	14.583	1922	1929	1939	rBV	1358246	1961809	15.56%	1.499%
19	14.689	1939	1947	1956	rBV	3260726	4782047	37.92%	3.655%
20	14.783	1956	1963	1981	rVB	2050314	3221249	25.54%	2.462%
21	15.207	2029	2035	2042	rVB	99936	148139	1.17%	0.113%
22	15.701	2112	2119	2130	rBV	1196208	1717813	13.62%	1.313%
23	16.066	2174	2181	2197	rBV	5011580	6842273	54.25%	5.230%
24	16.977	2329	2336	2355	rBV	6345030	8914501	70.68%	6.813%
25	17.324	2388	2395	2406	rBV	1562474	2240189	17.76%	1.712%
26	19.942	2834	2840	2854	rBV	10456065	12611786	100.00%	9.639%
27	21.495	3099	3104	3120	rBV	1517259	2222931	17.63%	1.699%
28	23.177	3387	3390	3399	rVB	129610	205190	1.63%	0.157%
29	23.812	3494	3498	3505	rVB	192564	324035	2.57%	0.248%
30	23.906	3508	3514	3526	rVV2	917445	2010864	15.94%	1.537%
31	24.547	3619	3623	3631	rVB2	173582	322383	2.56%	0.246%

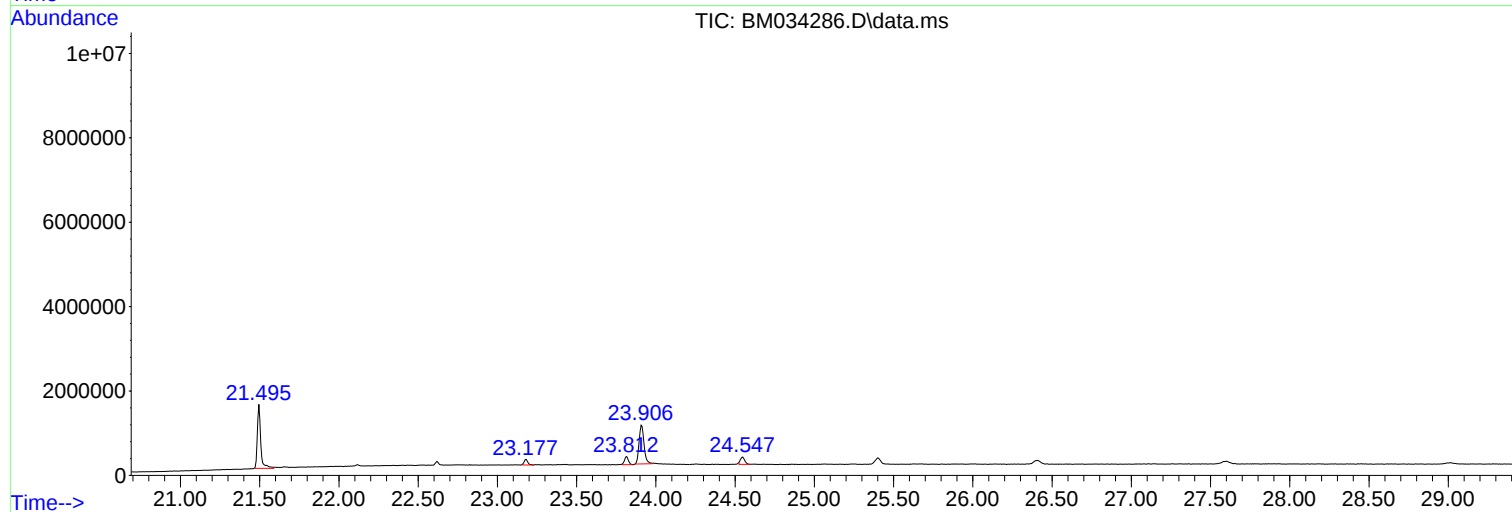
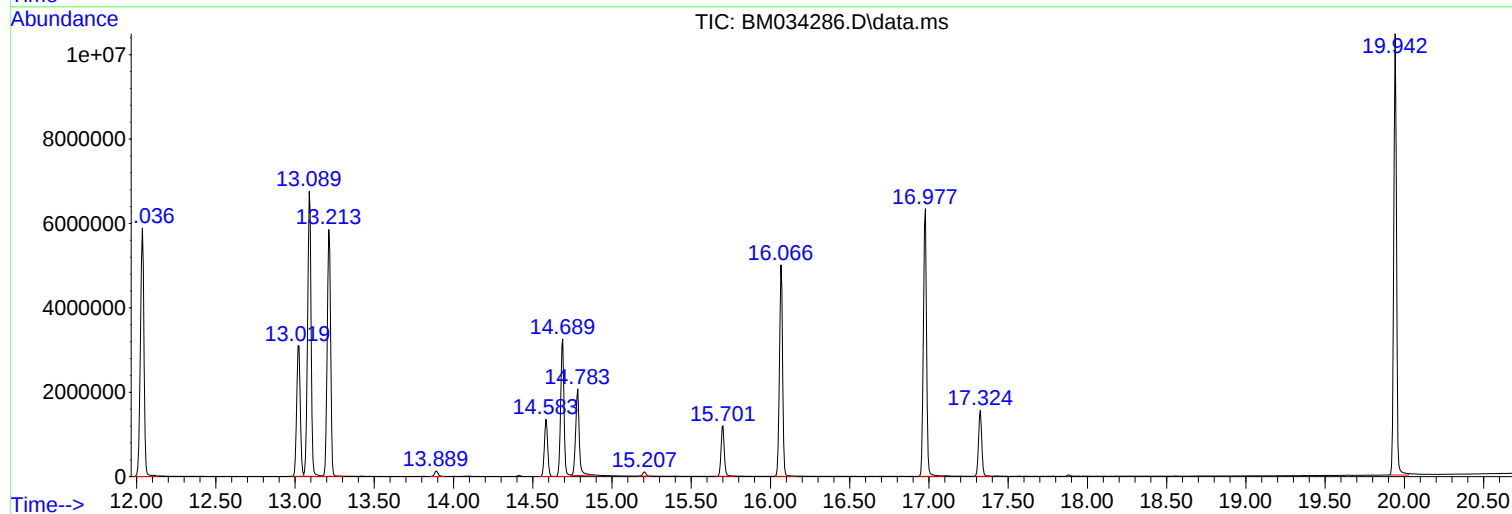
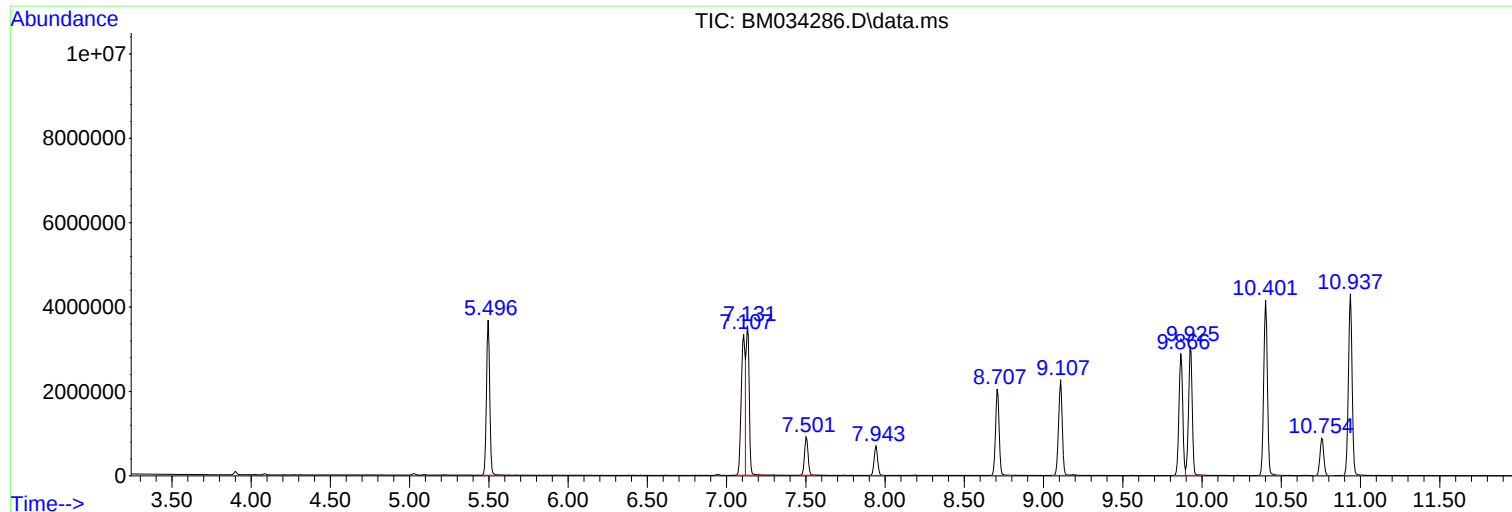
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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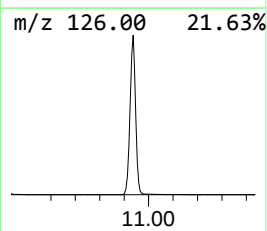
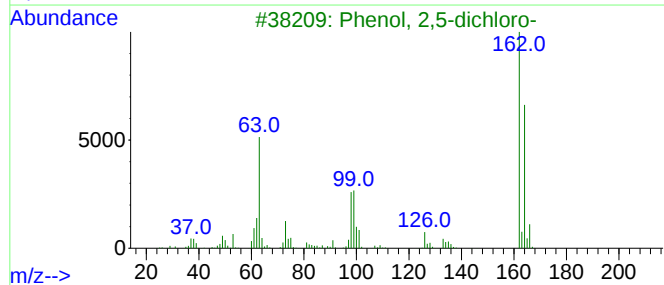
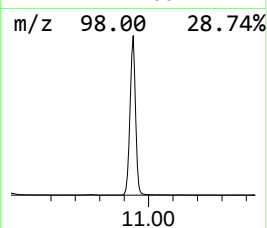
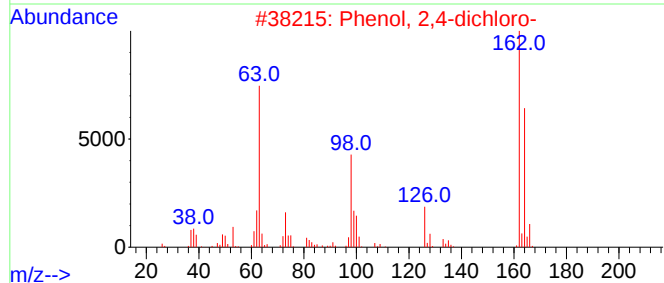
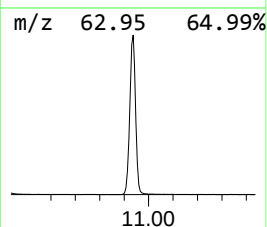
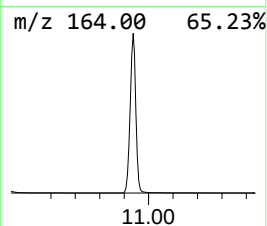
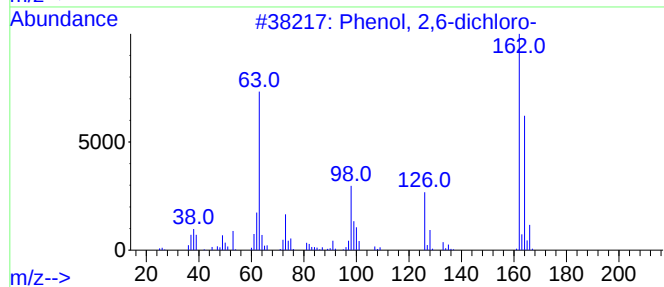
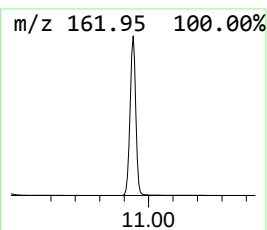
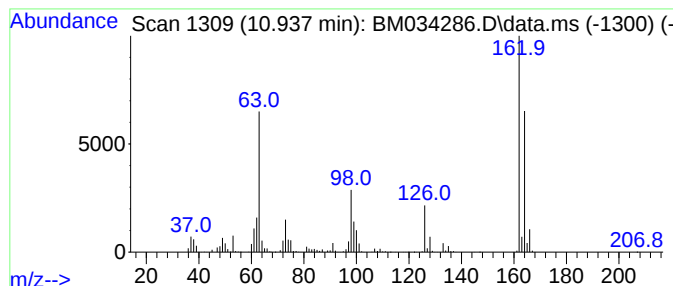
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Phenol, 2,6-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.937	95.11 ng	7044380	Naphthalene-d8	10.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-dichloro-	162	C6H4Cl2O	000087-65-0	98
2			Phenol, 2,4-dichloro-	162	C6H4Cl2O	000120-83-2	96
3			Phenol, 2,5-dichloro-	162	C6H4Cl2O	000583-78-8	94
4			Phenol, 2,3-dichloro-	162	C6H4Cl2O	000576-24-9	93
5			Phenol, 3,5-dichloro-	162	C6H4Cl2O	000591-35-5	64



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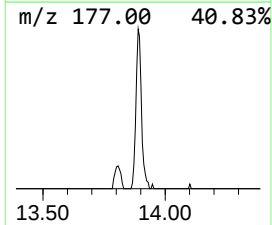
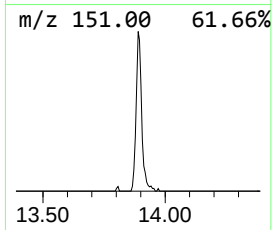
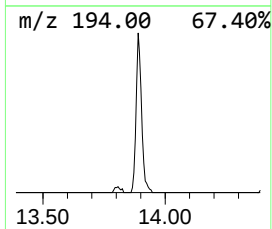
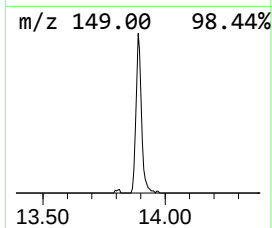
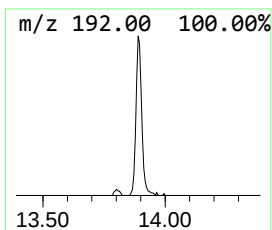
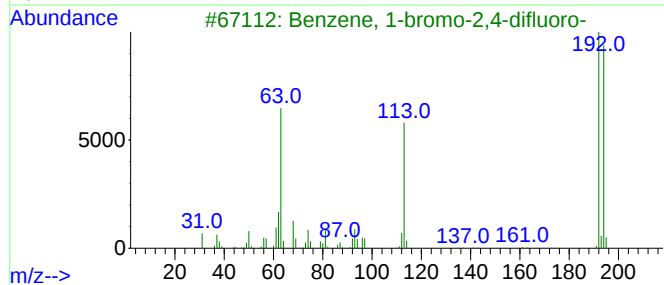
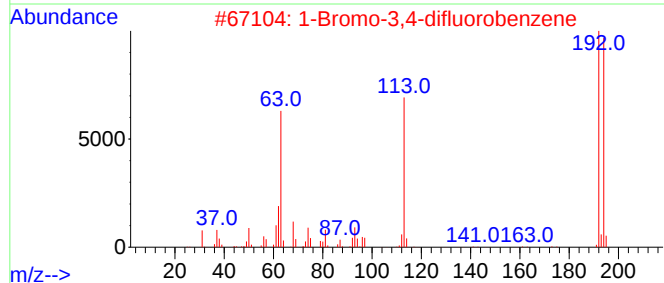
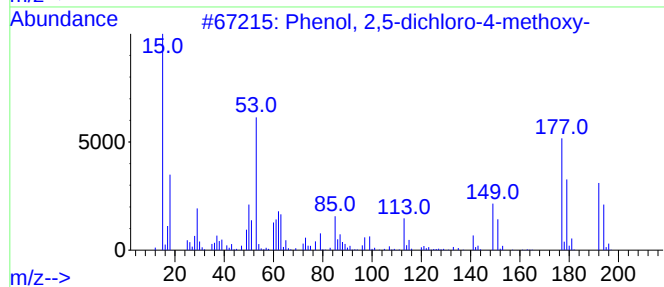
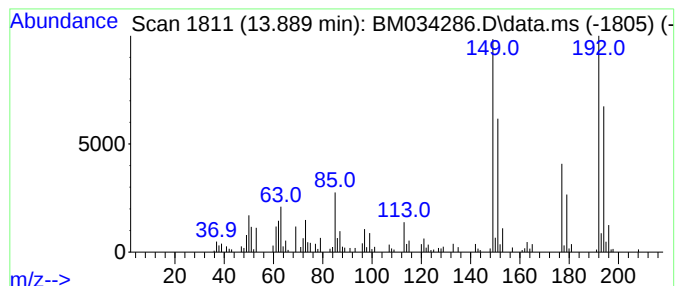
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown13.889 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.889	2.07 ng	202913	Acenaphthene-d10	14.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,5-dichloro-4-methoxy-	192	C7H6Cl2O2	018113-14-9	47
2			1-Bromo-3,4-difluorobenzene	192	C6H3BrF2	000348-61-8	38
3			Benzene, 1-bromo-2,4-difluoro-	192	C6H3BrF2	000348-57-2	30
4			6-Hydroxy-7-methoxycoumarin	192	C10H8O4	1000426-42-4	22
5			5-(Diethylamino)-2-nitrosophenol	194	C10H14N2O2	006358-20-9	18



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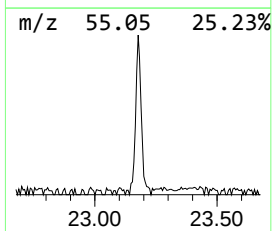
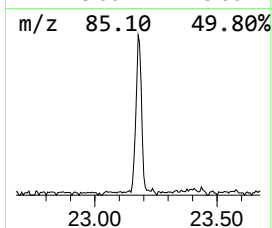
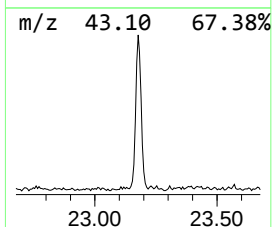
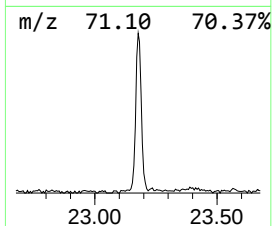
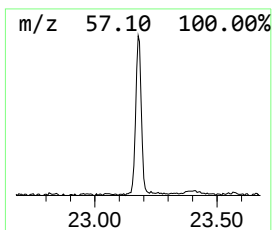
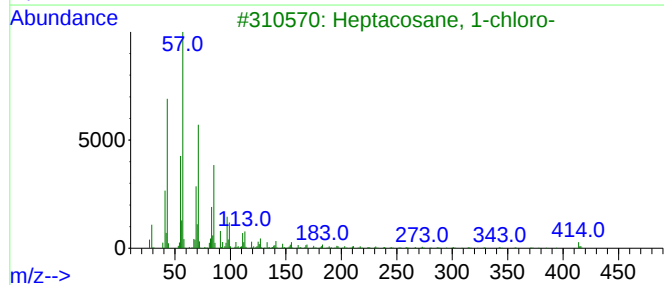
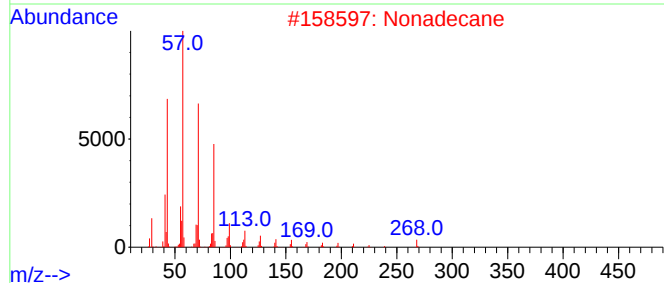
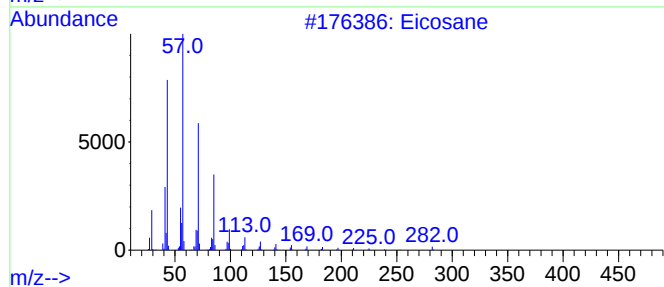
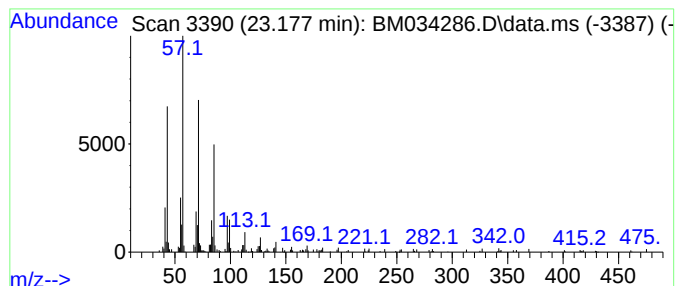
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.177	2.04 ng	205190	Perylene-d12	23.906

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Nonadecane	268	C19H40	000629-92-5	93
3			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Tetratetracontane	619	C44H90	007098-22-8	90



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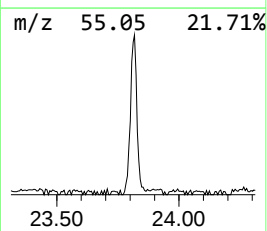
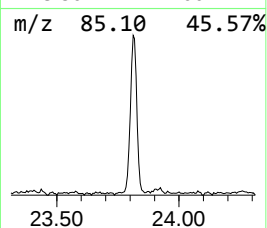
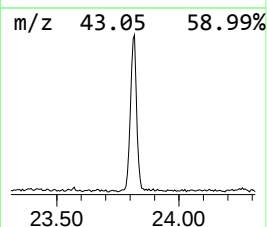
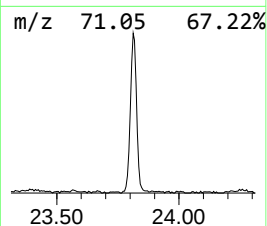
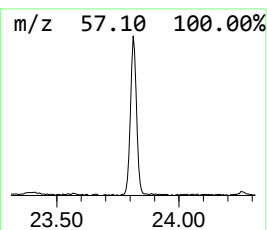
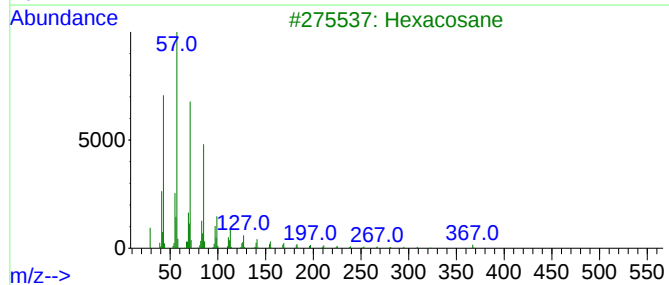
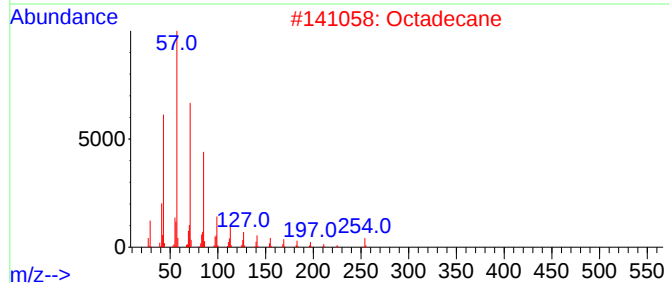
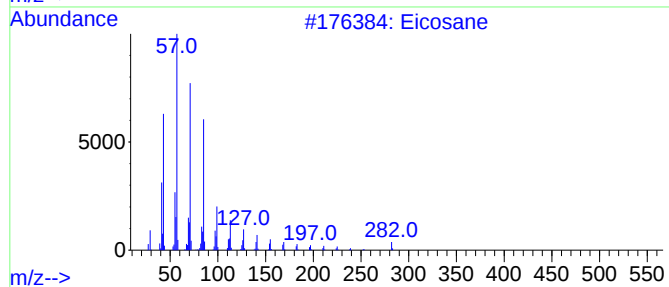
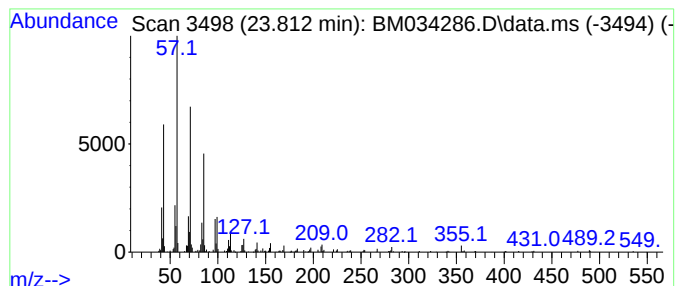
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Peak Number 4 Octadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.812	3.22 ng	324035	Perylene-d12	23.906

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Octadecane	254	C18H38	000593-45-3	93
3			Hexacosane	366	C26H54	000630-01-3	93
4			Octacosane	394	C28H58	000630-02-4	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



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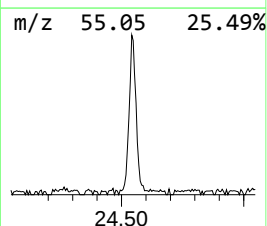
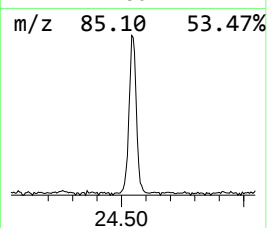
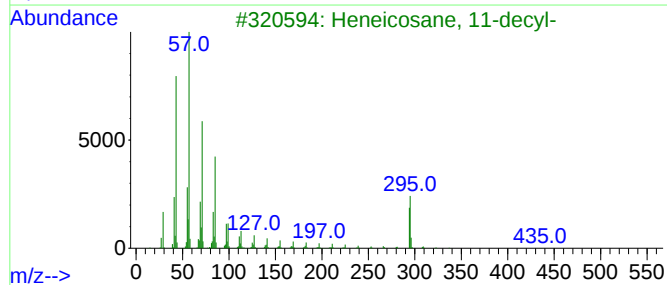
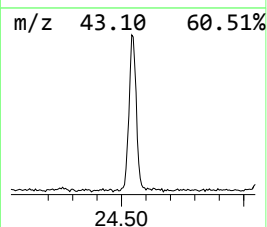
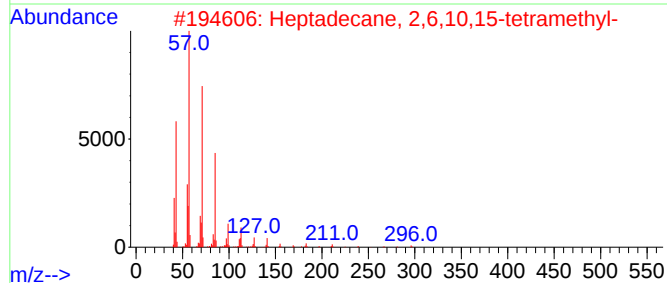
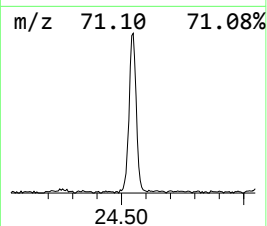
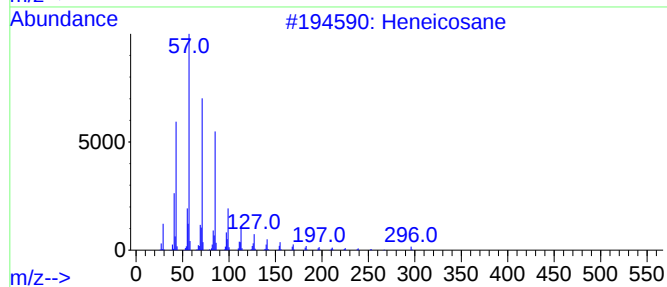
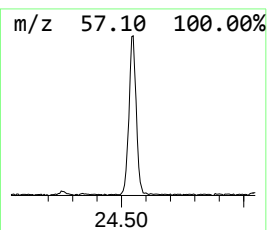
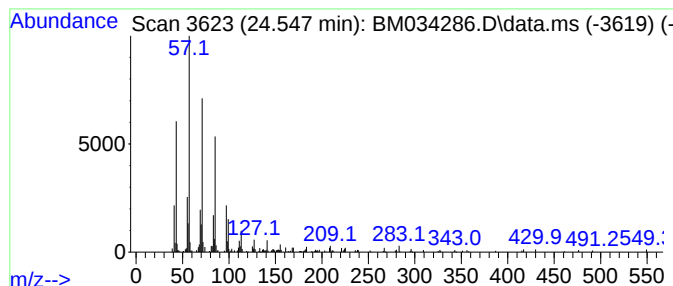
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.547	3.21 ng	322383	Perylene-d12	23.906

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	98
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	83
4			Hexatriacontane	507	C36H74	000630-06-8	83
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Phenol, 2,6-dic...	10.937	95.1	ng	7044380	2	10.754	1481350	20.0
unknown13.889	13.889	2.1	ng	202913	3	14.583	1961810	20.0
Eicosane	23.177	2.0	ng	205190	6	23.906	2010860	20.0
Octadecane	23.812	3.2	ng	324035	6	23.906	2010860	20.0
Heneicosane	24.547	3.2	ng	322383	6	23.906	2010860	20.0