

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
 Data File : BF126073.D
 Acq On : 8 Nov 2021 19:26
 Operator : JU/CG
 Sample : M4477-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T5-EP1-S

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_F\METHODS\8270-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126073.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	4	10	21	rVB	1961398	2403518	59.95%	8.180%
2	5.063	502	506	516	rVB	255895	296502	7.40%	1.009%
3	5.469	570	575	578	rBV	3809638	3347004	83.49%	11.391%
4	6.481	741	747	750	rBV	3291076	3569330	89.03%	12.148%
5	6.851	806	810	813	rBV	1308132	1019437	25.43%	3.470%
6	7.410	900	905	908	rBV	2336720	2318142	57.82%	7.890%
7	8.039	1007	1012	1024	rBV	1357323	1311291	32.71%	4.463%
8	8.133	1024	1028	1031	rVV	1531724	1207197	30.11%	4.109%
9	9.210	1206	1211	1214	rBV	4990010	4008978	100.00%	13.644%
10	9.886	1322	1326	1336	rBV	1497346	1223763	30.53%	4.165%
11	10.669	1456	1459	1474	rVB	1848175	1731686	43.20%	5.894%
12	11.369	1574	1578	1586	rBV	1241524	1042487	26.00%	3.548%
13	11.769	1642	1646	1649	rBV	122185	93243	2.33%	0.317%
14	12.474	1763	1766	1769	rVB	138091	108246	2.70%	0.368%
15	12.957	1843	1848	1851	rBV	4089917	3464373	86.42%	11.791%
16	13.498	1936	1940	1944	rBV	64781	67359	1.68%	0.229%
17	13.863	1998	2002	2016	rBV2	136657	265898	6.63%	0.905%
18	14.010	2023	2027	2035	rVB	1084022	1039064	25.92%	3.536%
19	15.468	2270	2275	2280	rBV	642158	803662	20.05%	2.735%
20	15.945	2353	2356	2362	rVB4	39111	61140	1.53%	0.208%

Sum of corrected areas: 29382320

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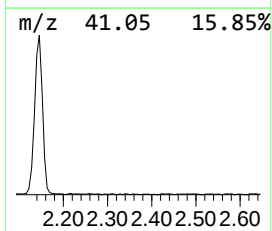
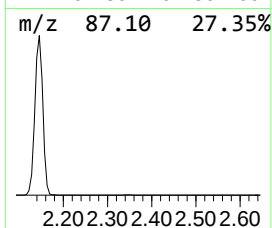
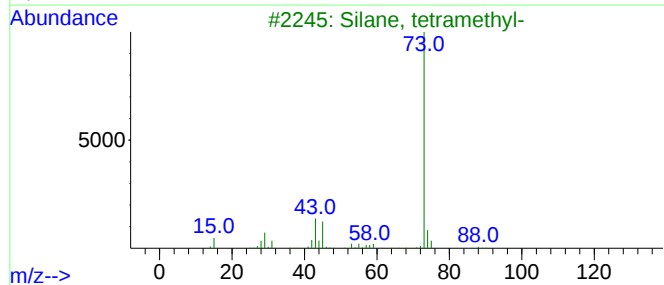
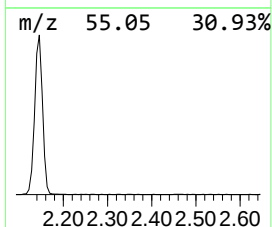
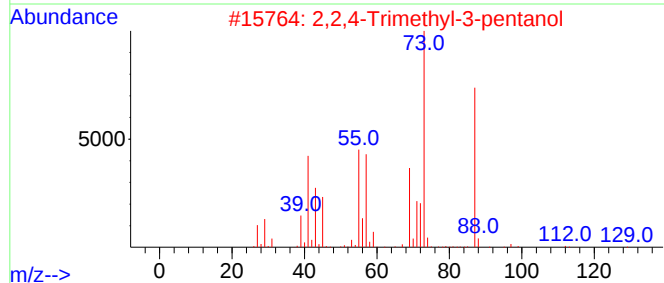
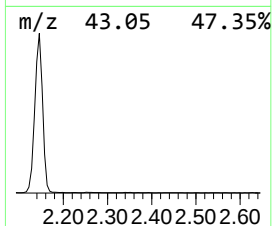
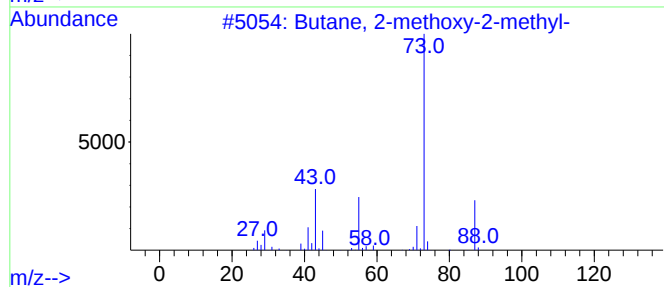
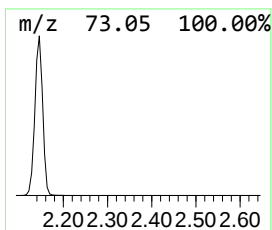
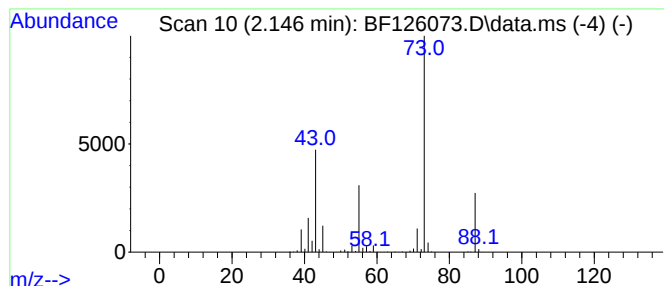
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	47.15 ng	2403520	1,4-Dichlorobenzene-d4	6.851

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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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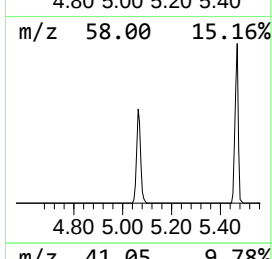
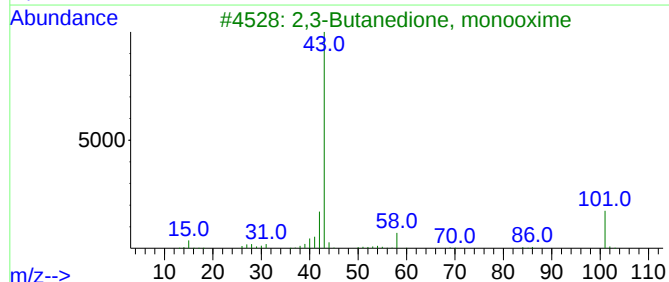
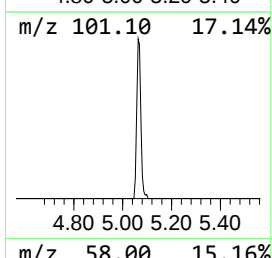
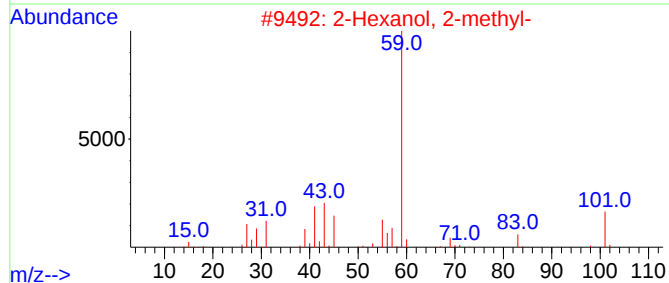
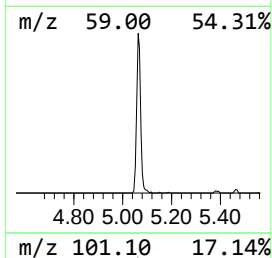
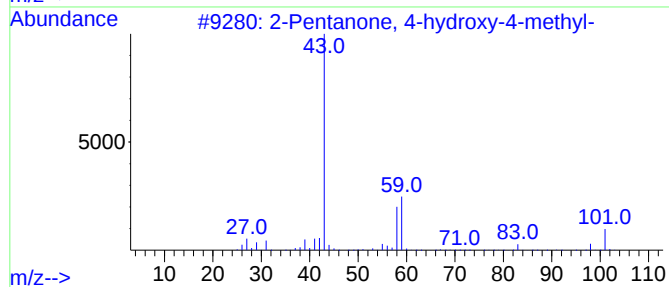
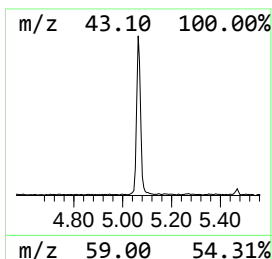
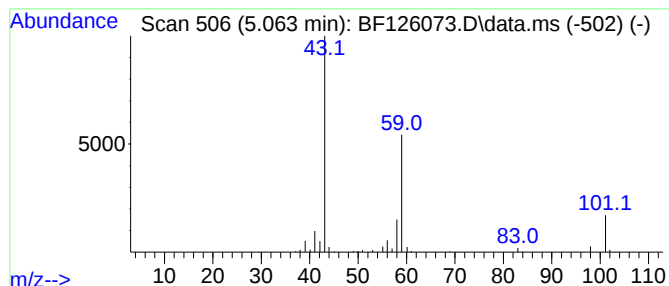
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	5.82 ng	296502	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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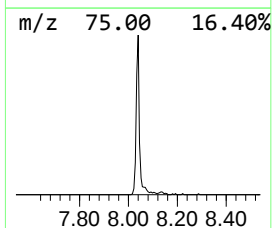
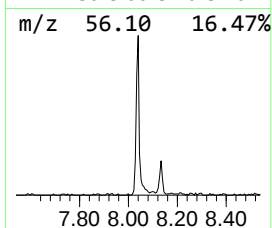
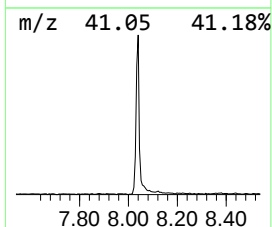
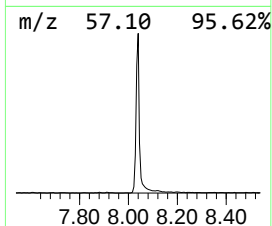
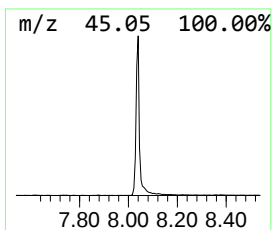
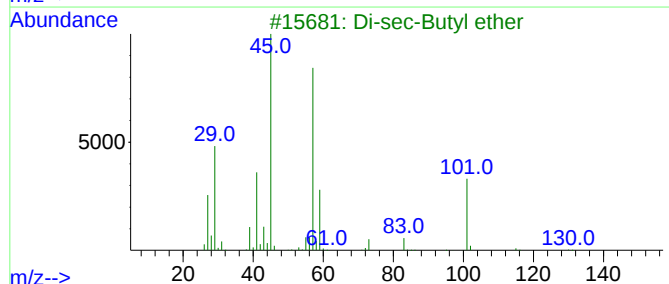
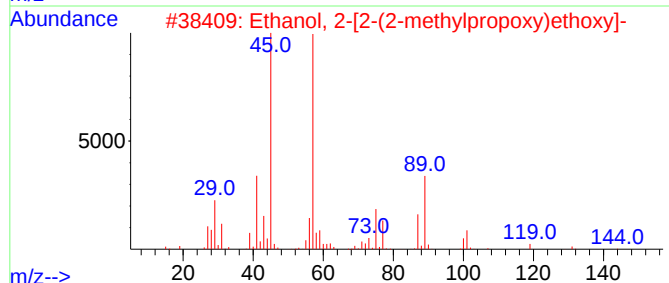
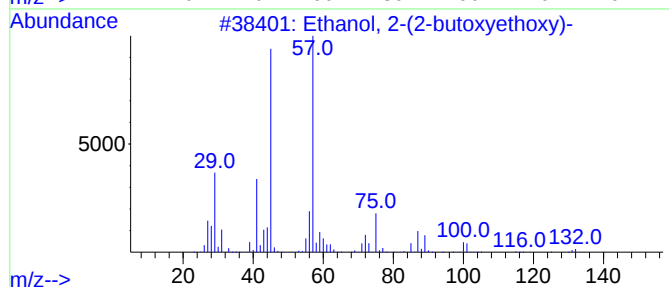
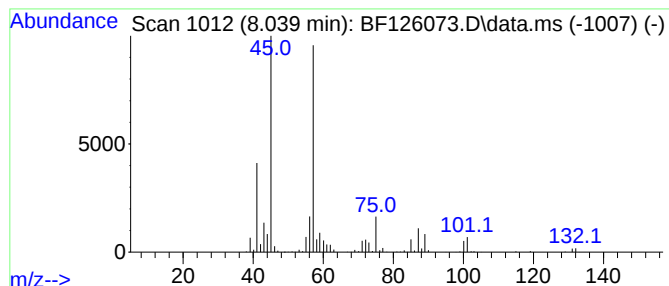
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	21.72 ng	1311290	Naphthalene-d8	8.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	52



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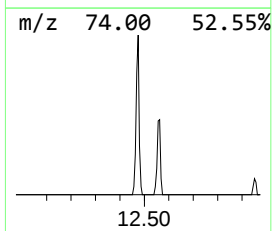
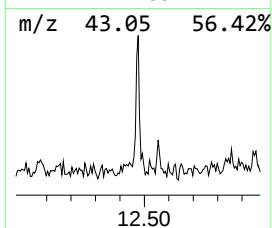
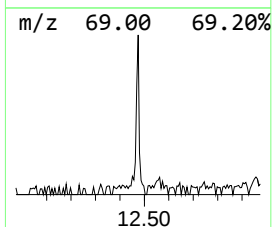
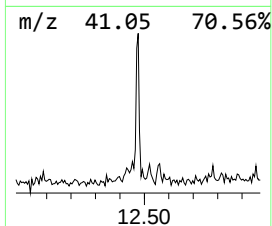
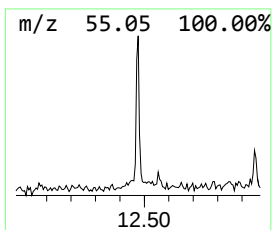
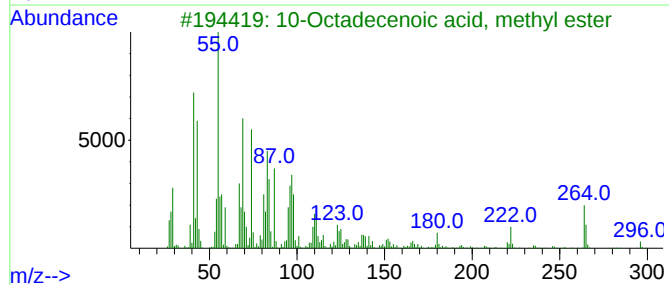
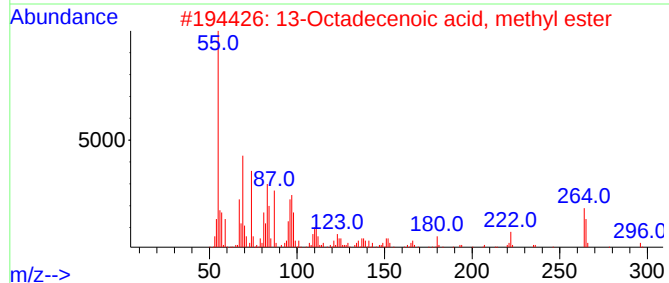
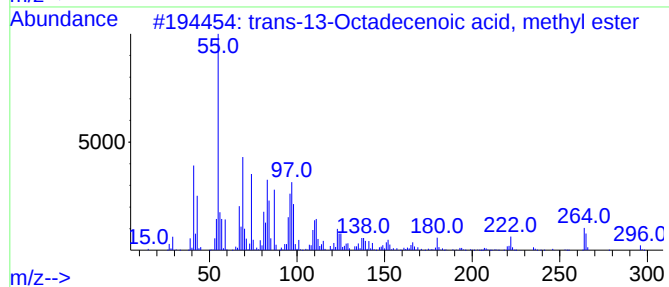
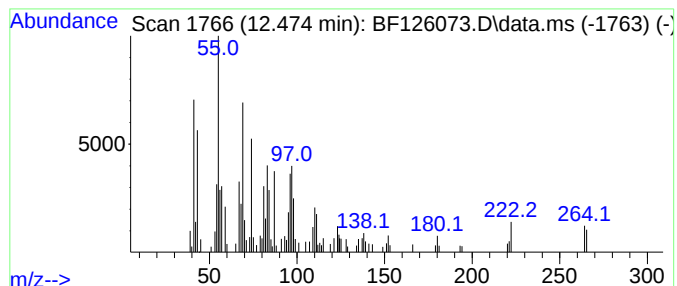
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Peak Number 4 trans-13-Octadecenoic acid,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.474	2.08 ng	108246	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
3			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4			Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	87
5			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	83



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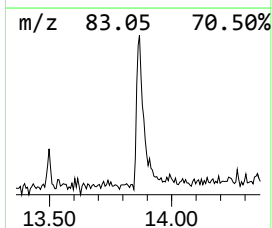
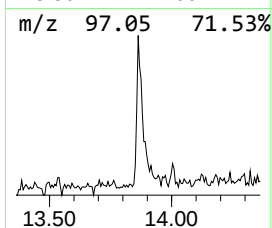
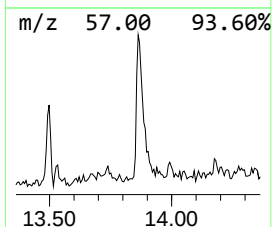
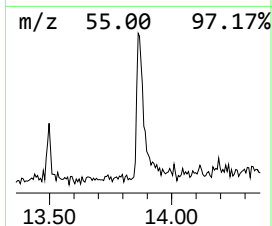
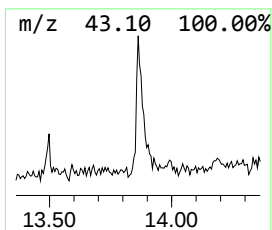
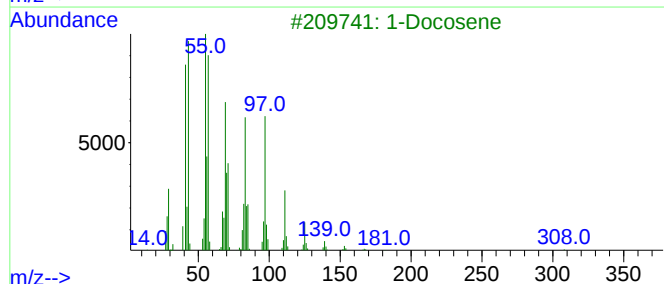
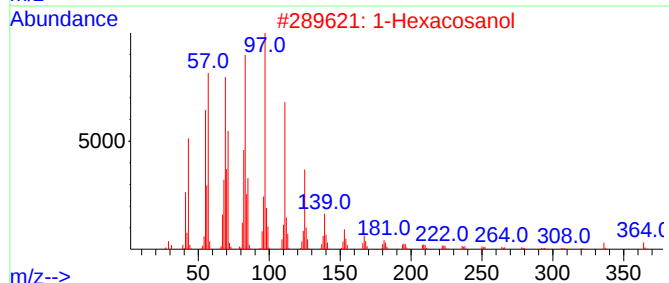
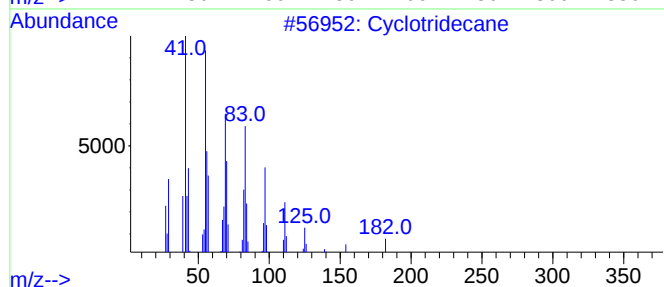
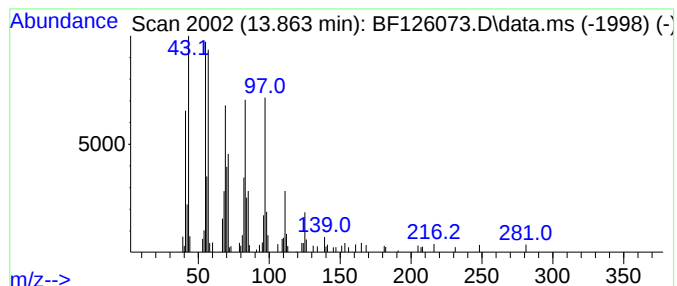
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Peak Number 5 Cyclotridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	5.12 ng	265898	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotridecane	182	C13H26	000295-02-3	93
2			1-Hexacosanol	382	C26H54O	000506-52-5	90
3			1-Docosene	308	C22H44	001599-67-3	90
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	47.1	ng	2403520	1	6.851	1019440	20.0
2-Pentanone, 4-...	5.063	5.8	ng	296502	1	6.851	1019440	20.0
Ethanol, 2-(2-b...	8.039	21.7	ng	1311290	2	8.133	1207200	20.0
trans-13-Octade...	12.474	2.1	ng	108246	4	11.369	1042490	20.0
Cyclotridecane	13.863	5.1	ng	265898	5	14.010	1039060	20.0