

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062221\
 Data File : BP006021.D
 Acq On : 23 Jun 2021 00:12
 Operator : CG/JU
 Sample : M2773-06
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-6

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-BP060821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006021.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.493	402	409	427	rBV	773705	1241972	37.58%	6.401%
2	7.093	674	681	701	rBV	689161	1204285	36.44%	6.207%
3	7.916	814	821	831	rBV	250163	407878	12.34%	2.102%
4	9.087	1009	1020	1034	rBV	409109	750459	22.71%	3.868%
5	10.446	1245	1251	1256	rBV2	13826	33584	1.02%	0.173%
6	10.510	1256	1262	1291	rVV	111574	295968	8.95%	1.525%
7	10.722	1291	1298	1310	rVB	318176	551523	16.69%	2.842%
8	11.987	1503	1513	1524	rBV3	16263	42939	1.30%	0.221%
9	13.175	1707	1715	1732	rBV	1259474	1891192	57.22%	9.747%
10	13.969	1841	1850	1857	rBV3	17646	34676	1.05%	0.179%
11	14.545	1941	1948	1963	rBV	491791	739117	22.36%	3.809%
12	16.034	2195	2201	2222	rBV	992750	1614591	48.85%	8.321%
13	17.122	2376	2386	2391	rBV2	291433	542099	16.40%	2.794%
14	17.292	2409	2415	2427	rBV	611644	1068958	32.34%	5.509%
15	17.957	2524	2528	2534	rVB	36845	42352	1.28%	0.218%
16	18.175	2560	2565	2570	rBV	57711	83402	2.52%	0.430%
17	19.080	2716	2719	2724	rVB2	50458	56927	1.72%	0.293%
18	19.398	2769	2773	2780	rBV3	32616	52715	1.59%	0.272%
19	19.839	2843	2848	2856	rBV	2695310	3305230	100.00%	17.034%
20	21.075	3054	3058	3064	rBV	120671	203578	6.16%	1.049%
21	21.363	3102	3107	3120	rBV	901383	1289867	39.03%	6.648%
22	21.986	3209	3213	3224	rBV2	411974	832201	25.18%	4.289%
23	23.074	3392	3398	3419	rVB	741587	1736488	52.54%	8.949%
24	23.768	3509	3516	3529	rVB2	644435	1381337	41.79%	7.119%

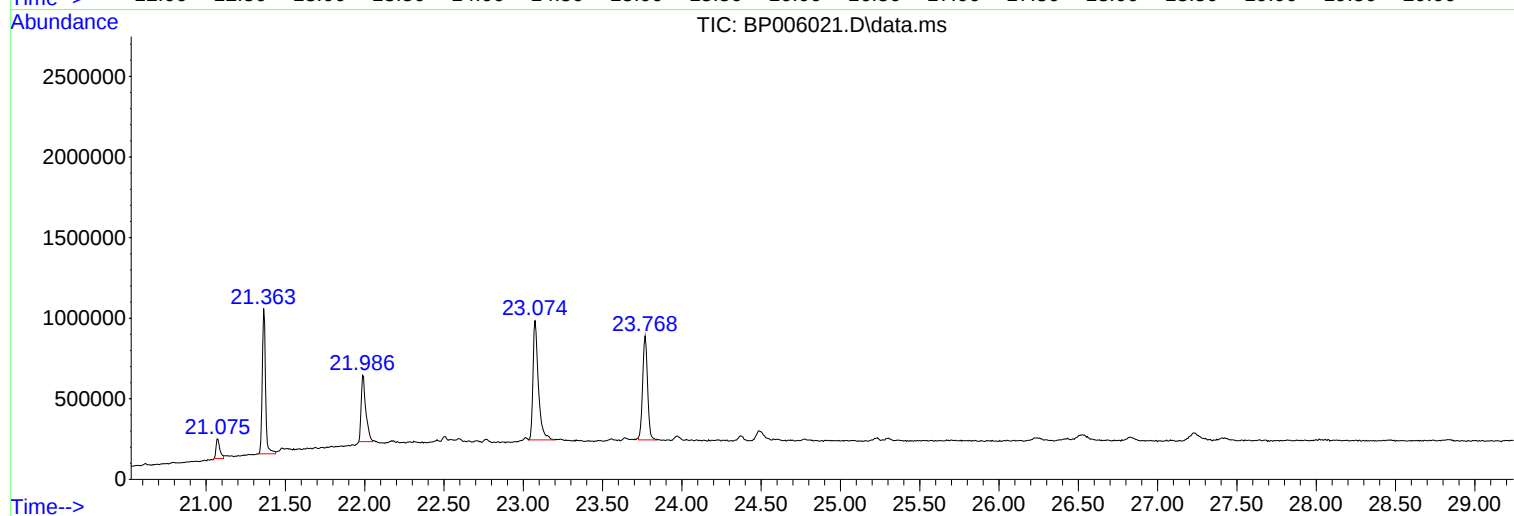
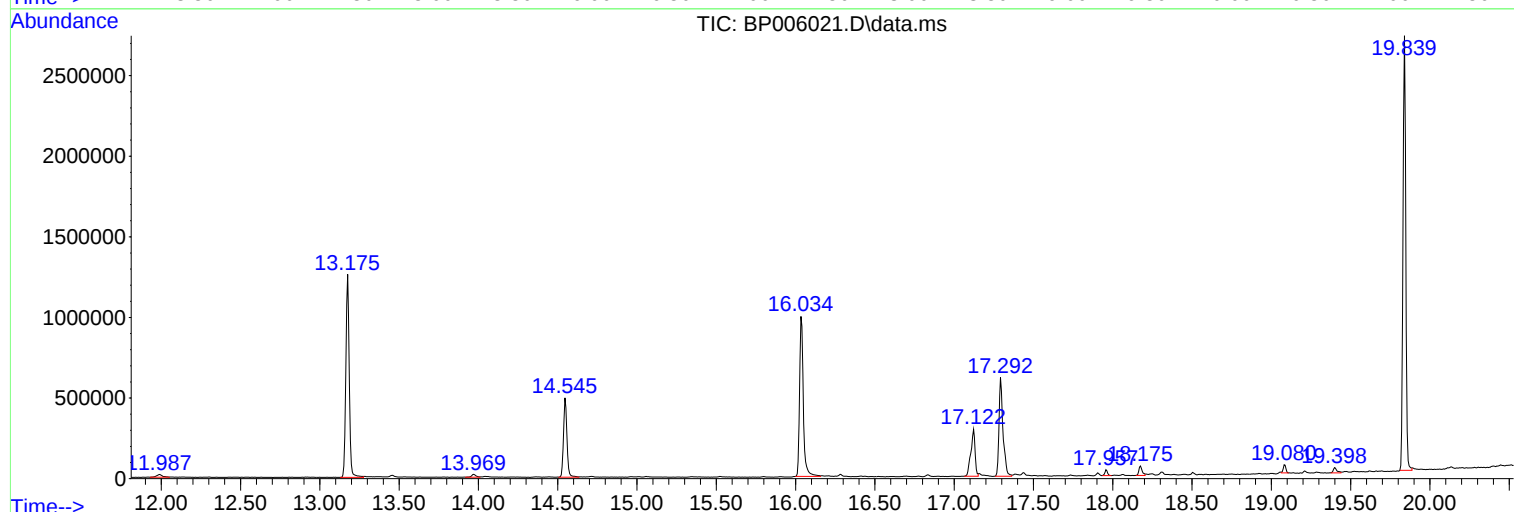
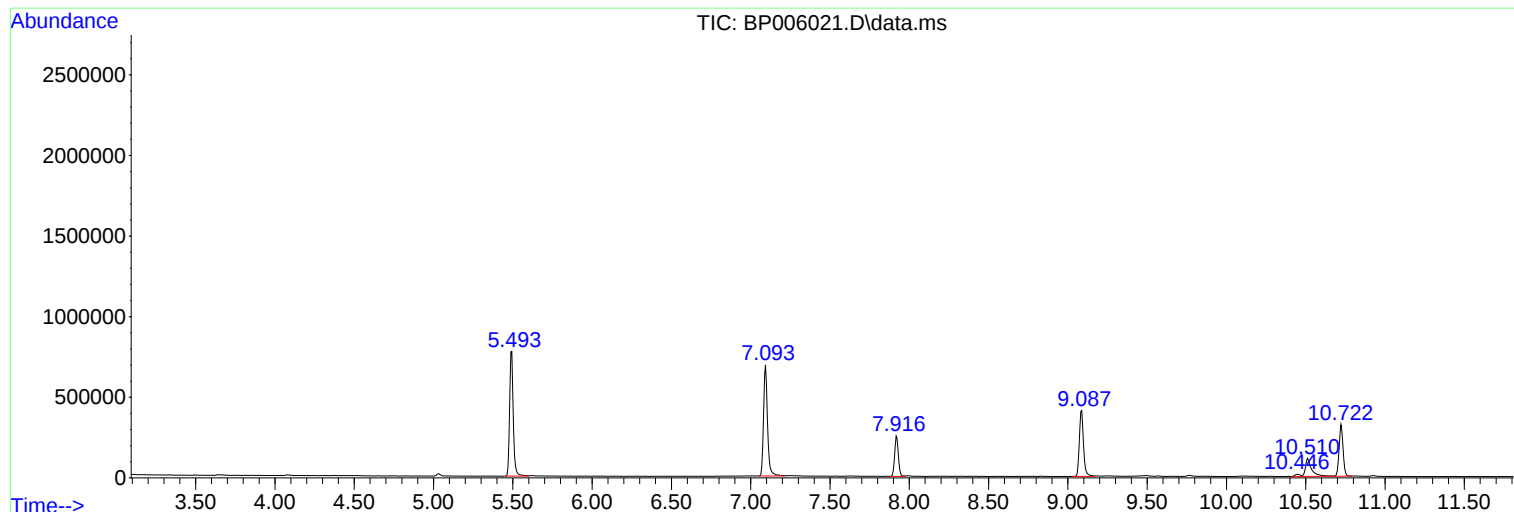
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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Misc :
ALS Vial : 15 Sample Multiplier: 1

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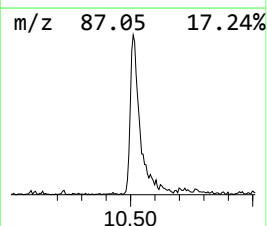
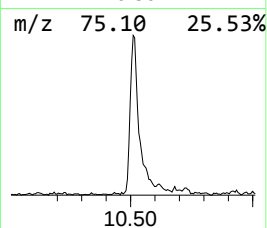
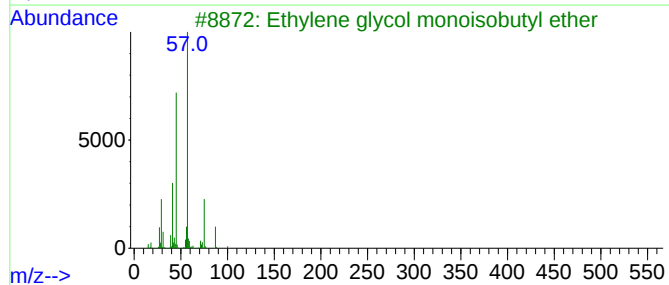
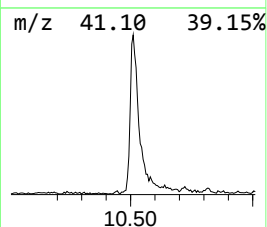
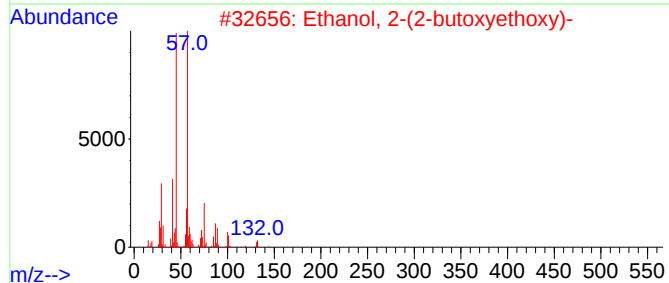
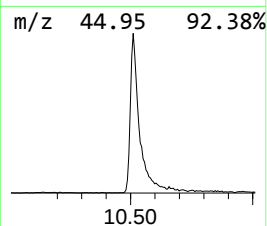
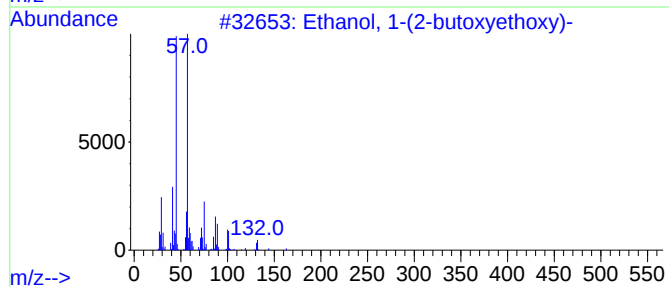
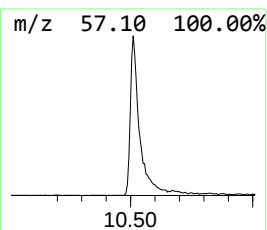
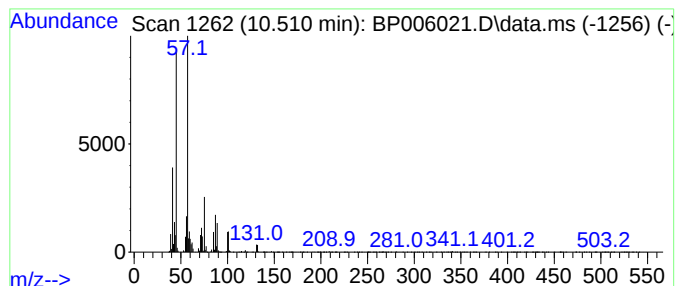
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.510	10.73 ng	295968	Naphthalene-d8	10.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	49
5			Triethylene glycol	150	C6H14O4	000112-27-6	47



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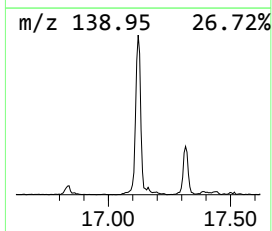
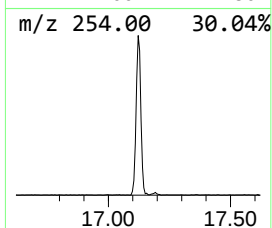
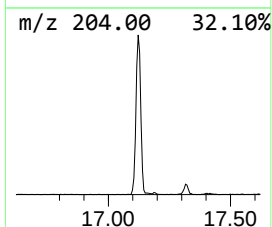
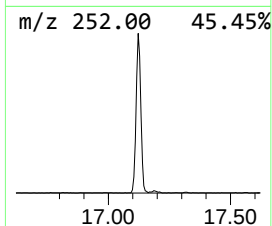
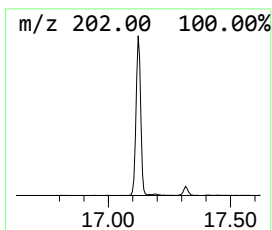
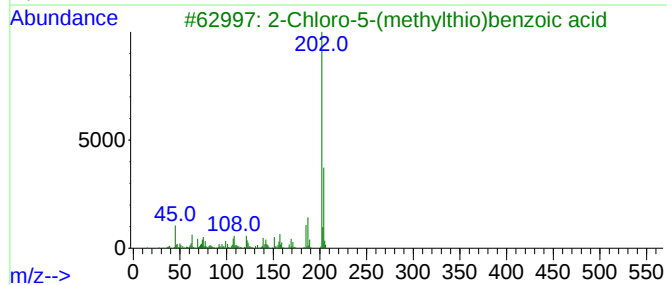
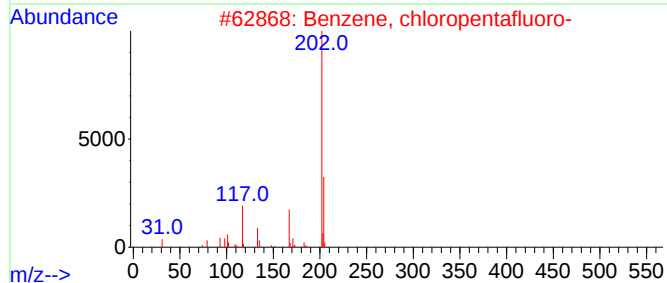
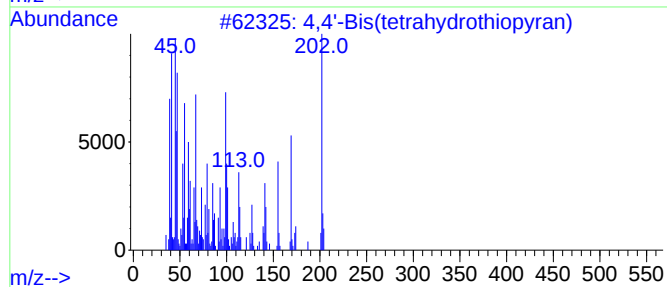
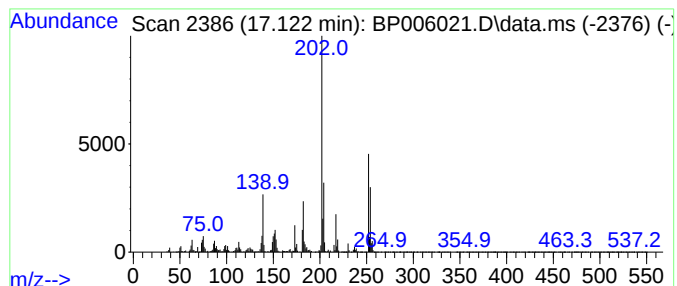
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown17.122 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.122	10.14 ng	542099	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	38
2			Benzene, chloropentafluoro-	202	C6ClF5	000344-07-0	35
3			2-Chloro-5-(methylthio)benzoic acid	202	C8H7ClO2S	051546-12-4	35
4			1,2,3-Thiadiazole, 4-(4-trifluor...	230	C9H5F3N2S	253122-65-5	35
5			Cyclopropane-1,1-dicarbonitrile,...	202	C11H7ClN2	098235-21-3	32



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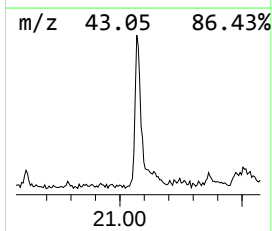
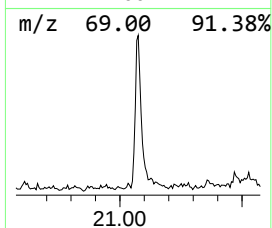
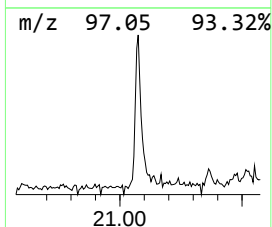
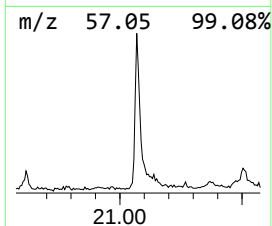
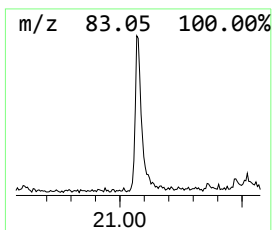
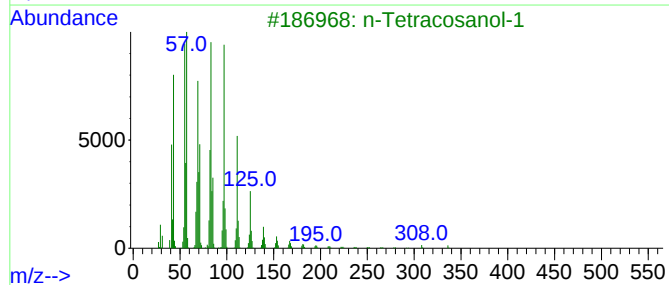
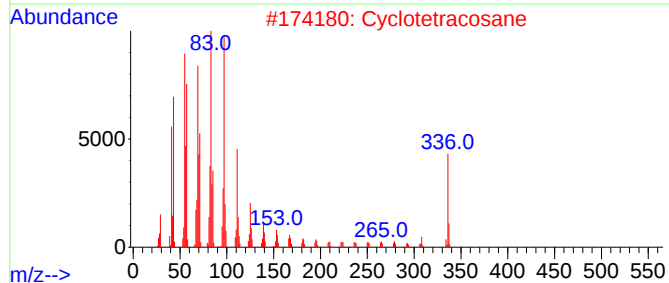
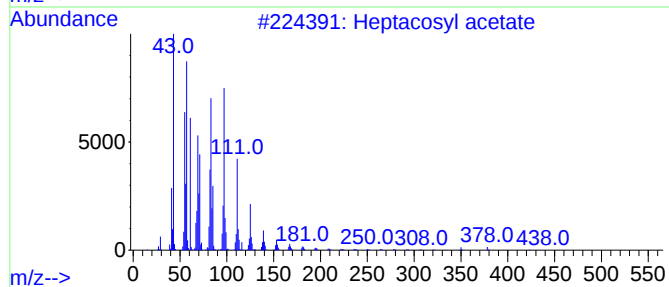
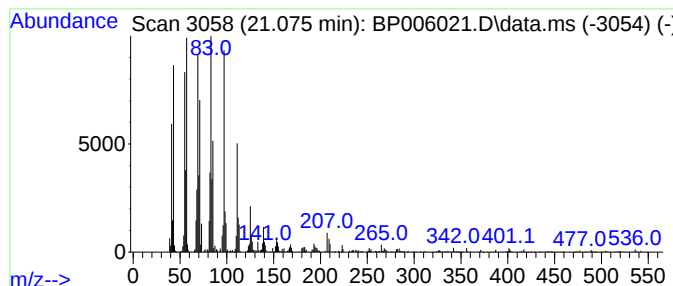
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptacosyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.075	3.16 ng	203578	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	94
2			Cyclotetracosane	336	C24H48	000297-03-0	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4			Triacetyl acetate	480	C32H64O2	041755-58-2	90
5			Cyclopentadecane	210	C15H30	000295-48-7	89



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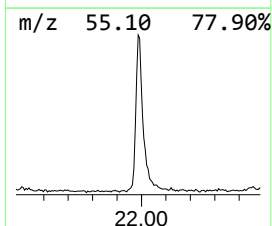
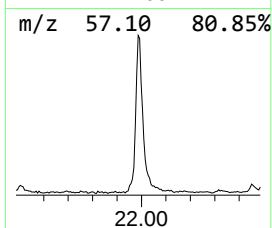
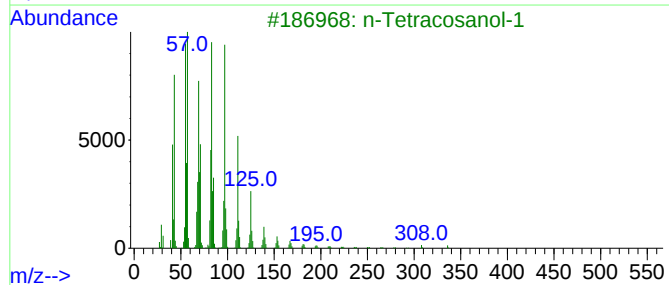
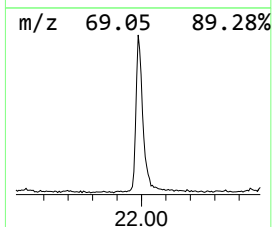
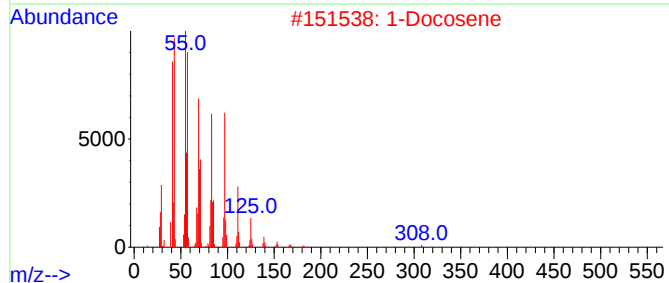
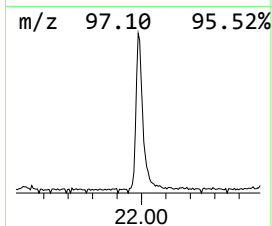
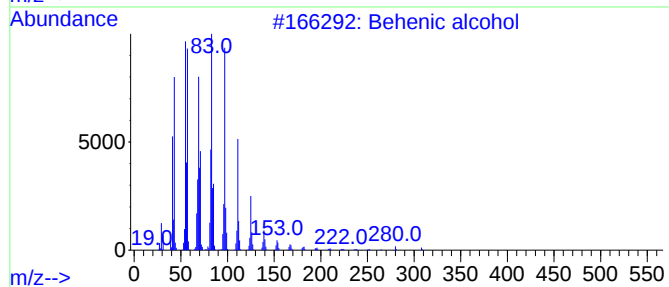
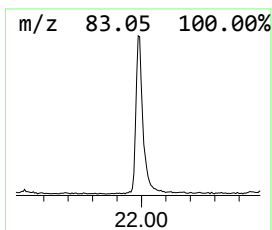
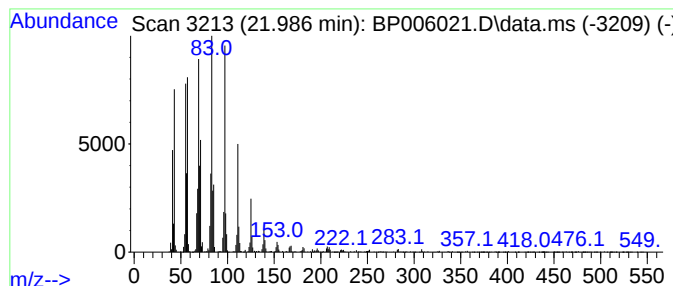
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.986	12.90 ng	832201	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			1-Docosene	308	C22H44	001599-67-3	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5			1-Heptacosanol	396	C27H56O	002004-39-9	93



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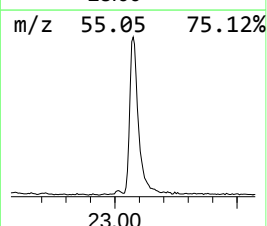
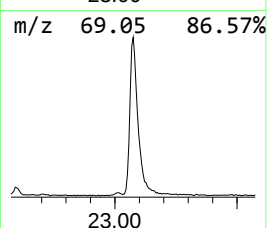
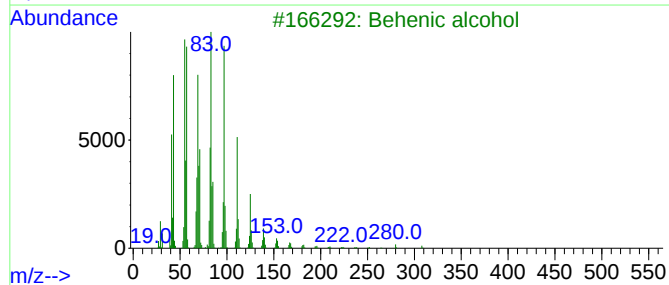
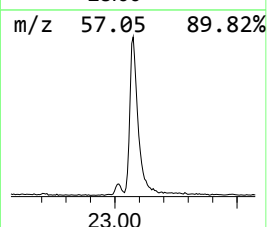
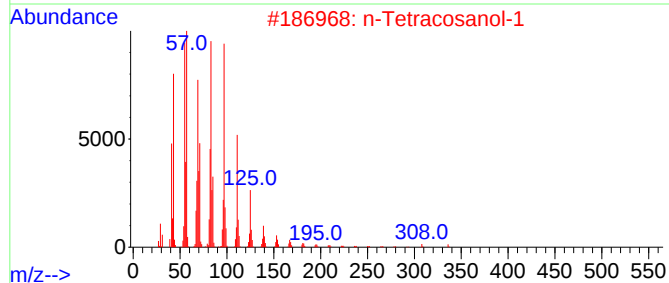
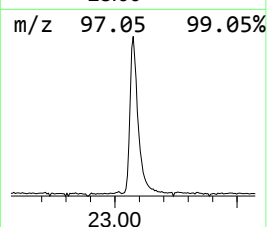
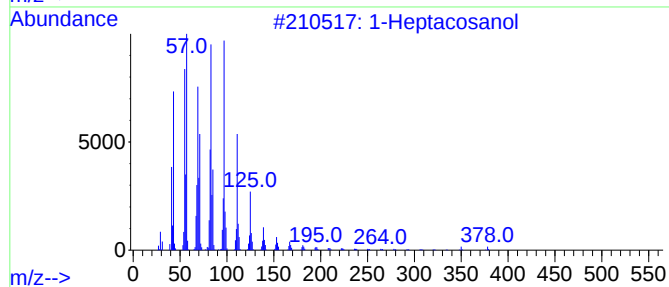
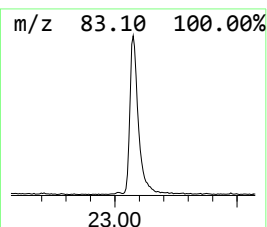
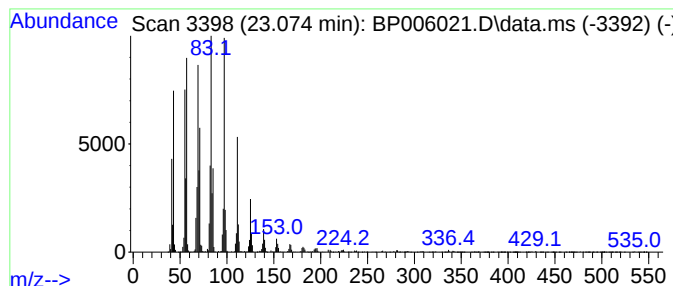
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Heptacosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.074	25.14 ng	1736490	Perylene-d12	23.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			Octacosanol	410	C28H58O	000557-61-9	93
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 1-(2-b...	10.510	10.7	ng	295968	2	10.722	551523	20.0
unknown17.122	17.122	10.1	ng	542099	4	17.292	1068960	20.0
Heptacosyl acetate	21.075	3.2	ng	203578	5	21.363	1289870	20.0
Behenic alcohol	21.986	12.9	ng	832201	5	21.363	1289870	20.0
1-Heptacosanol	23.074	25.1	ng	1736490	6	23.769	1381340	20.0