

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
 Data File : BF125278.D
 Acq On : 30 Aug 2021 23:42
 Operator : JU/CG
 Sample : M3569-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-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_F\METHODS\8270-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125278.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	10	15	29	rVB	1103141	1421737	32.46%	4.154%
2	5.145	515	520	529	rVB	61501	83679	1.91%	0.245%
3	5.540	582	587	590	rBV	3949127	3734416	85.26%	10.912%
4	6.551	754	759	762	rBV	3945933	3757114	85.78%	10.978%
5	6.916	817	821	824	rBV	1336334	1039155	23.72%	3.036%
6	7.481	912	917	920	rBV	2874789	2489097	56.83%	7.273%
7	8.098	1019	1022	1029	rBV	467110	545097	12.45%	1.593%
8	8.169	1032	1034	1036	rVV	67499	61206	1.40%	0.179%
9	8.198	1036	1039	1046	rVB	1700170	1392687	31.80%	4.069%
10	8.610	1106	1109	1111	rBV	74272	60350	1.38%	0.176%
11	8.781	1135	1138	1142	rVB	163439	128612	2.94%	0.376%
12	9.210	1209	1211	1217	rVB	66156	51887	1.18%	0.152%
13	9.275	1217	1222	1225	rBV	4877528	4380004	100.00%	12.798%
14	9.345	1231	1234	1237	rBV	137125	112000	2.56%	0.327%
15	9.663	1285	1288	1291	rBV3	79444	81236	1.85%	0.237%
16	9.875	1319	1324	1328	rBV	116720	102537	2.34%	0.300%
17	9.951	1334	1337	1341	rBV	1820855	1585899	36.21%	4.634%
18	10.192	1375	1378	1383	rBV4	39136	48605	1.11%	0.142%
19	10.375	1406	1409	1411	rVB	126733	98686	2.25%	0.288%
20	10.592	1443	1446	1452	rVB	87806	103105	2.35%	0.301%
21	10.745	1468	1472	1482	rVB	3133178	2941746	67.16%	8.596%
22	10.845	1486	1489	1490	rBV	146631	115836	2.64%	0.338%
23	11.298	1563	1566	1568	rBV	113464	100957	2.30%	0.295%
24	11.327	1568	1571	1577	rVB3	105400	139902	3.19%	0.409%
25	11.445	1587	1591	1593	rBV	1633350	1556811	35.54%	4.549%
26	11.463	1593	1594	1598	rVV	330918	244464	5.58%	0.714%
27	11.516	1600	1603	1605	rVB	65451	59674	1.36%	0.174%
28	11.722	1635	1638	1641	rBV	104339	86952	1.99%	0.254%
29	11.822	1653	1655	1658	rBV	74749	61093	1.39%	0.179%
30	11.957	1674	1678	1684	rBV2	228863	297422	6.79%	0.869%
31	12.057	1692	1695	1697	rBV2	62573	69212	1.58%	0.202%
32	12.133	1705	1708	1713	rBV	68730	74008	1.69%	0.216%
33	12.521	1771	1774	1778	rBV2	70693	72435	1.65%	0.212%
34	12.657	1794	1797	1800	rBV	544126	445876	10.18%	1.303%
35	12.745	1810	1812	1816	rBV4	56939	61427	1.40%	0.179%
36	12.886	1831	1836	1839	rBV	523779	526366	12.02%	1.538%

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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_F\METHODS\8270-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.027	1856	1860	1863	rBV	4119098	3486506	79.60%	10.187%
38	13.921	2009	2012	2017	rBV2	237208	281905	6.44%	0.824%
39	14.086	2035	2040	2042	rBV2	1169764	1259060	28.75%	3.679%
40	14.110	2042	2044	2047	rVB	193352	156322	3.57%	0.457%
41	15.592	2292	2296	2302	rBV	684682	908688	20.75%	2.655%

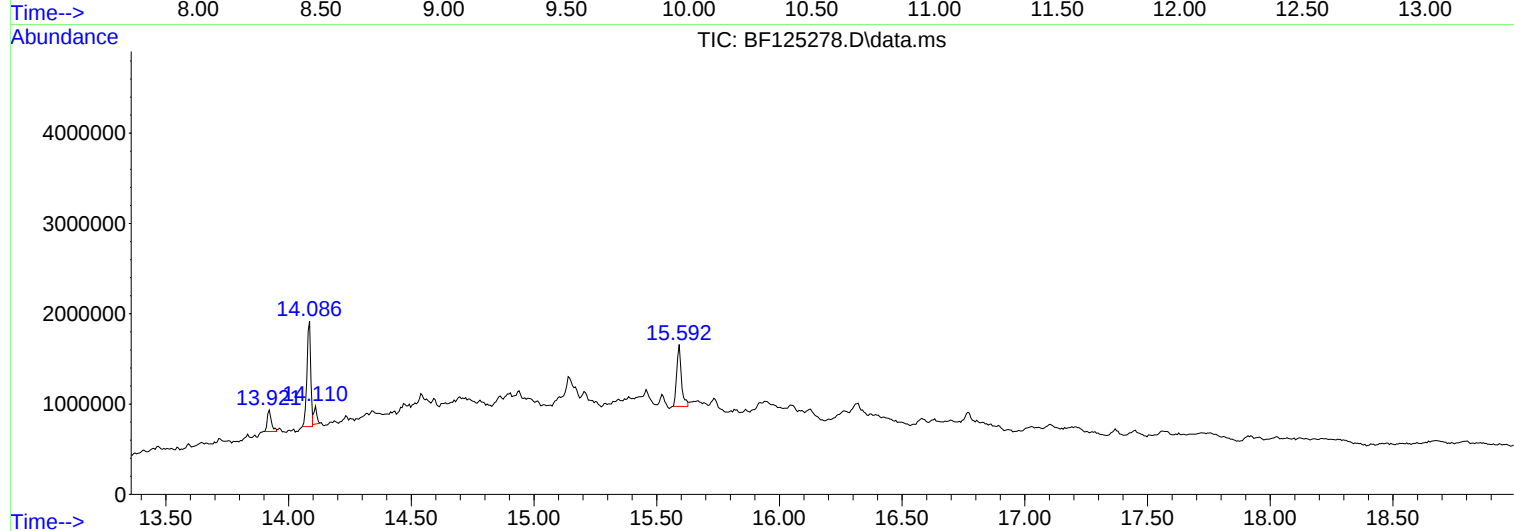
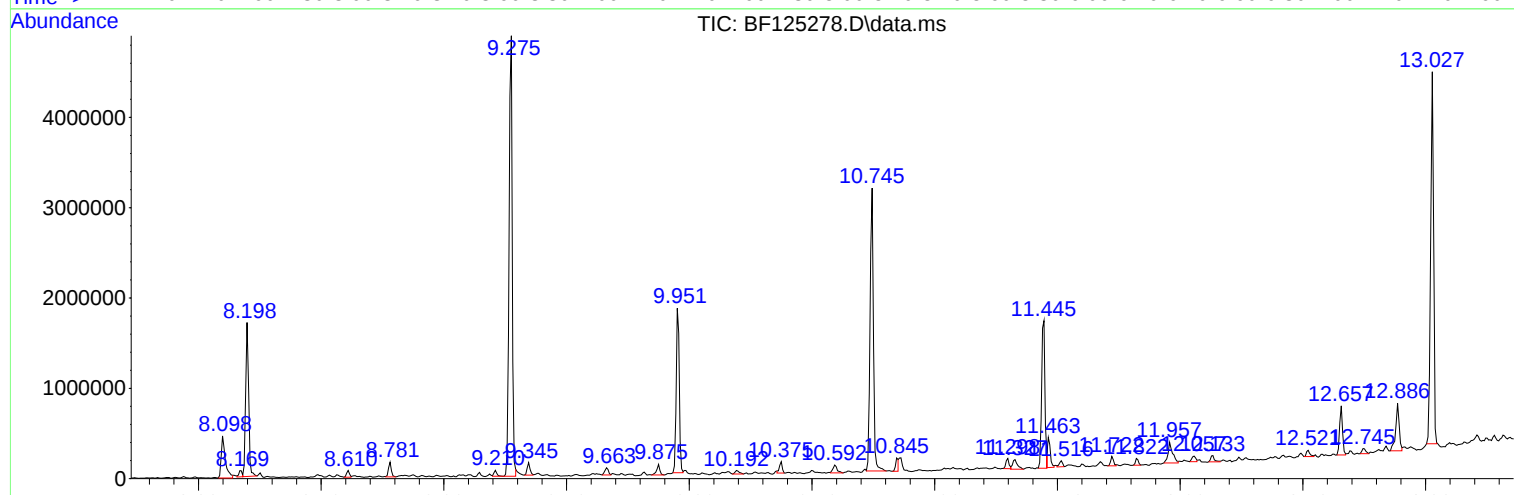
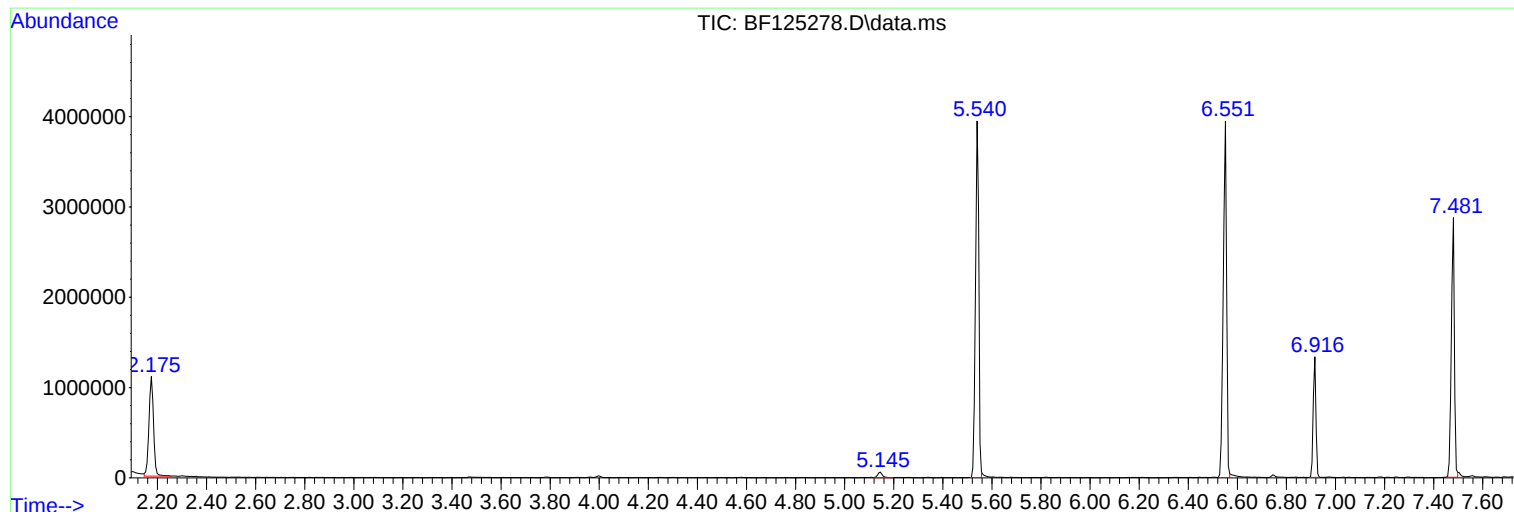
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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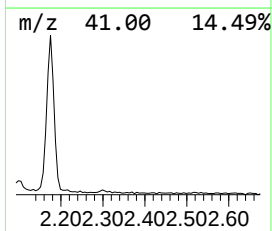
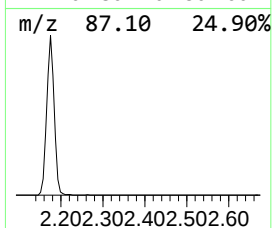
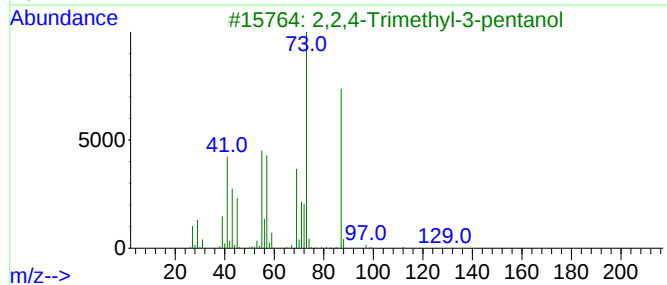
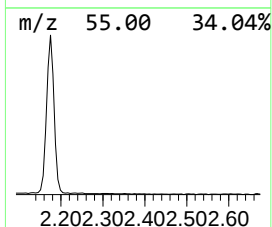
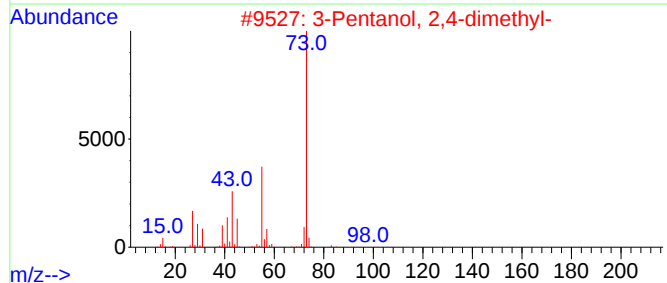
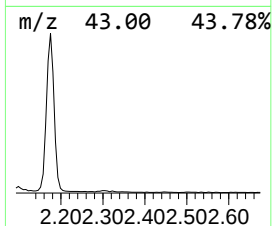
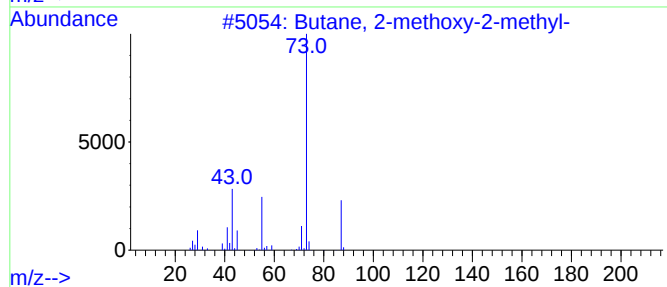
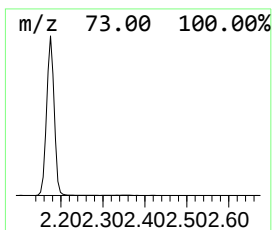
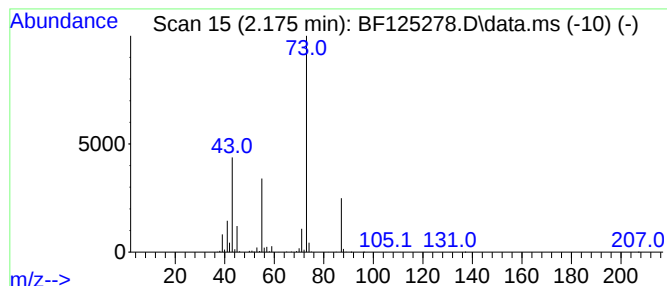
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.175	27.36 ng	1421740	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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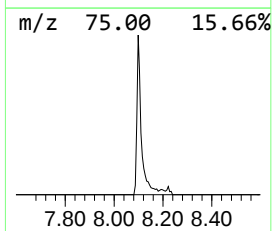
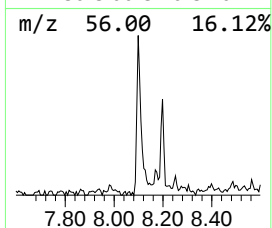
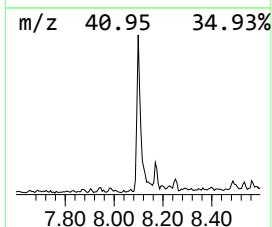
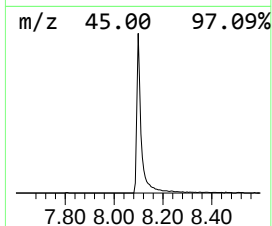
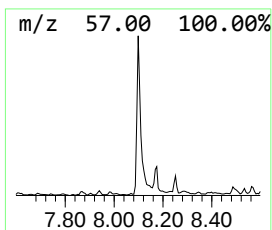
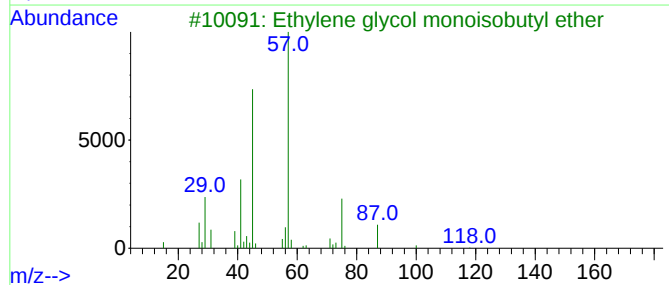
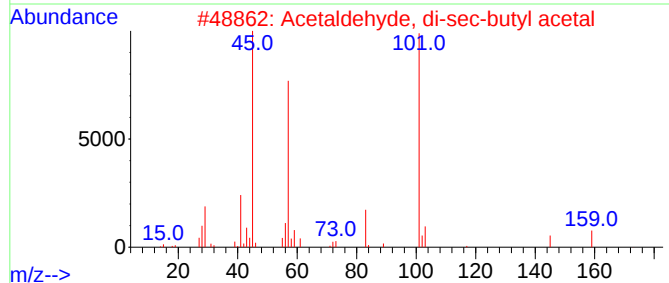
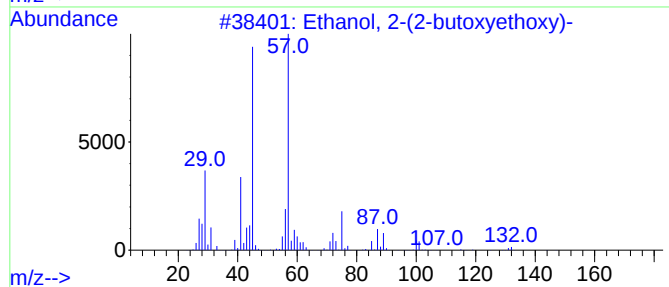
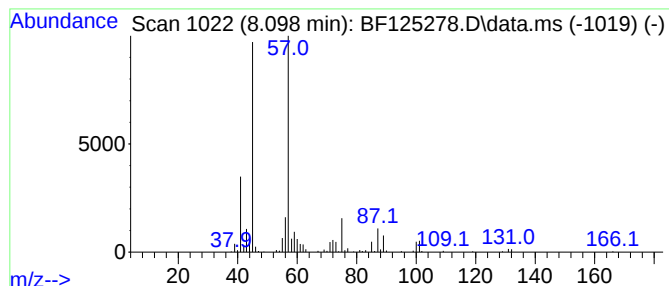
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	7.83 ng	545097	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	59
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56



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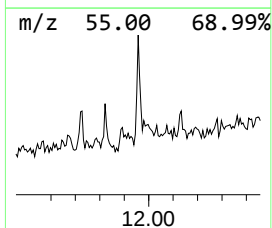
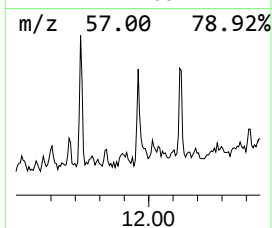
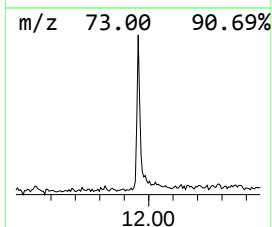
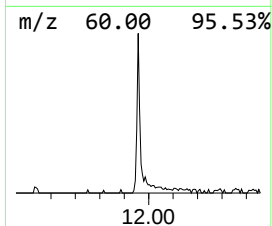
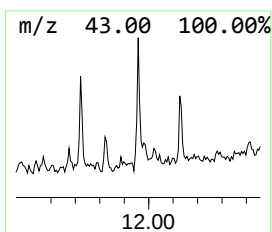
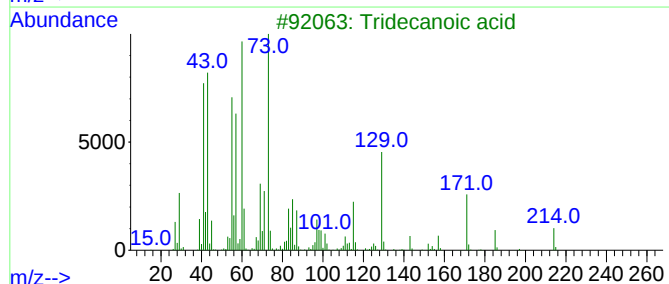
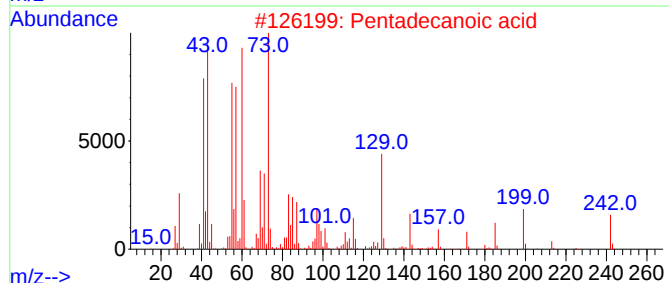
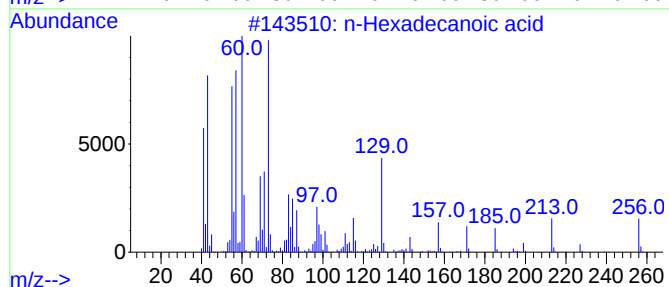
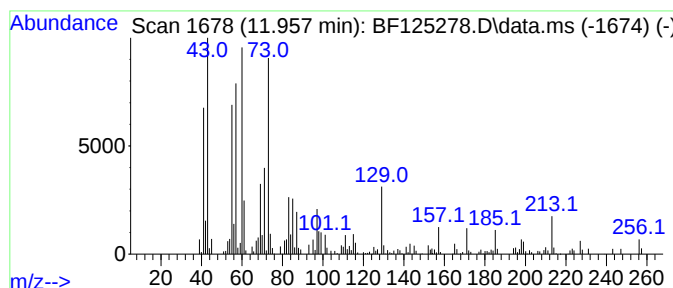
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	3.82 ng	297422	Phenanthrene-d10	11.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Undecanoic acid	186	C11H22O2	000112-37-8	83



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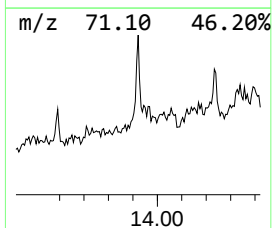
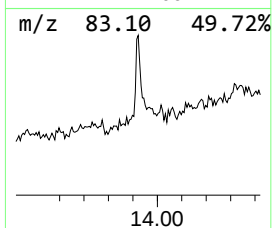
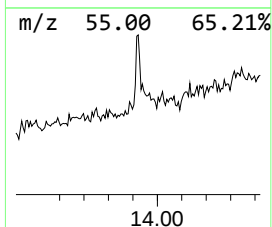
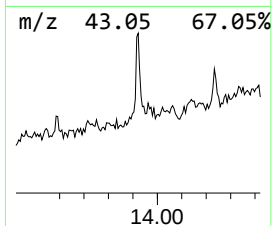
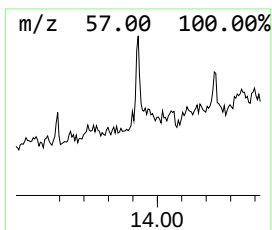
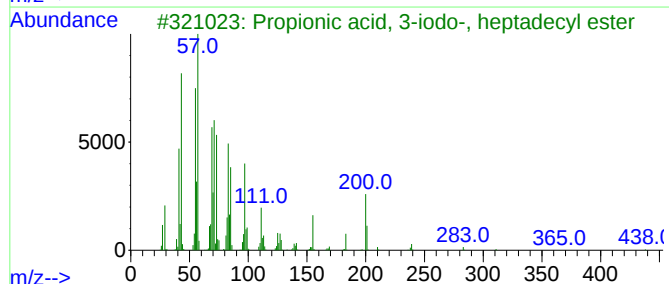
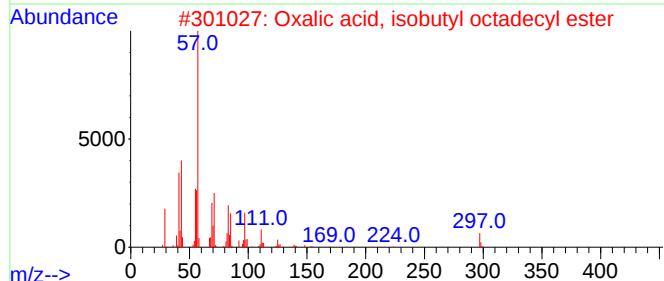
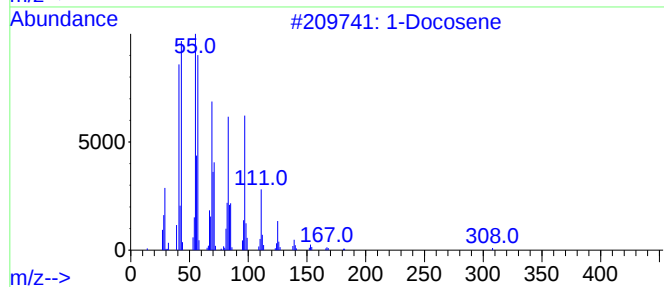
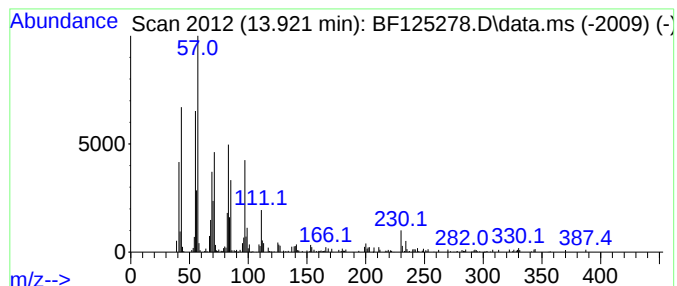
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Peak Number 4 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	4.48 ng	281905	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	89
2	Oxalic acid, isobutyl octadecyl ...			398	C24H46O4	1000309-38-3	87
3	Propionic acid, 3-iodo-, heptade...			438	C20H39IO2	1000406-24-8	87
4	Octacosyl trifluoroacetate			506	C30H57F3O2	1000351-74-9	87
5	Oxalic acid, isobutyl hexadecyl ...			370	C22H42O4	1000309-38-1	87



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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
Butane, 2-metho...	2.175	27.4	ng	1421740	1	6.916	1039160	20.0
Ethanol, 2-(2-b...	8.098	7.8	ng	545097	2	8.198	1392690	20.0
n-Hexadecanoic ...	11.957	3.8	ng	297422	4	11.445	1556810	20.0
1-Docosene	13.921	4.5	ng	281905	5	14.086	1259060	20.0