

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083121\
 Data File : BF125283.D
 Acq On : 31 Aug 2021 11:59
 Operator : JU/CG
 Sample : M3561-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OUII-C

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: BF125283.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	12	19	24	rVB	3692922	5028442	59.68%	10.988%
2	5.534	582	586	589	rBV	2932809	2587840	30.71%	5.655%
3	6.539	753	757	768	rBV	1946433	1697702	20.15%	3.710%
4	6.910	817	820	824	rBV	1331780	1148381	13.63%	2.509%
5	7.481	911	917	920	rBV	3812508	3694223	43.85%	8.072%
6	8.098	1018	1022	1035	rBV	807581	1068539	12.68%	2.335%
7	8.198	1035	1039	1042	rBV	1816937	1512379	17.95%	3.305%
8	9.275	1217	1222	1225	rBV	6679157	6341691	75.27%	13.857%
9	9.951	1333	1337	1346	rVB	2170025	1833297	21.76%	4.006%
10	10.327	1398	1401	1404	rBV	121234	105791	1.26%	0.231%
11	10.745	1467	1472	1475	rBV	4866174	4718750	56.01%	10.311%
12	11.439	1586	1590	1594	rBV	2415638	1999771	23.74%	4.370%
13	11.821	1652	1655	1658	rVB	205261	162050	1.92%	0.354%
14	11.957	1673	1678	1683	rBV	709953	745623	8.85%	1.629%
15	12.745	1808	1812	1820	rBV	376506	407413	4.84%	0.890%
16	13.033	1855	1861	1864	rBV	7873815	8425382	100.00%	18.410%
17	13.557	1946	1950	1952	rBV	95798	102202	1.21%	0.223%
18	13.945	2012	2016	2023	rVB	273741	369076	4.38%	0.806%
19	14.080	2035	2039	2043	rBV	2139472	1930608	22.91%	4.219%
20	14.933	2181	2184	2189	rVB	121869	115138	1.37%	0.252%
21	15.580	2288	2294	2306	rBV	1209868	1770713	21.02%	3.869%

Sum of corrected areas: 45765011

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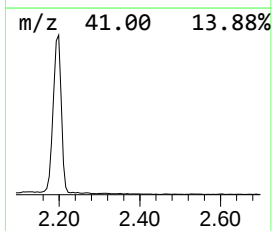
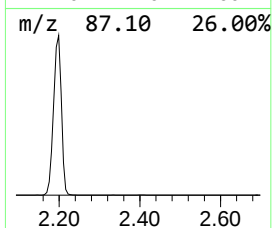
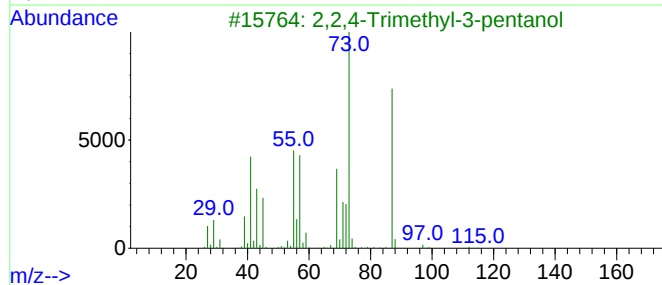
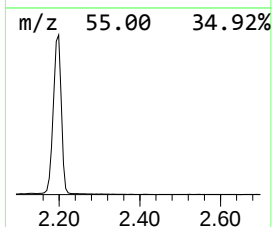
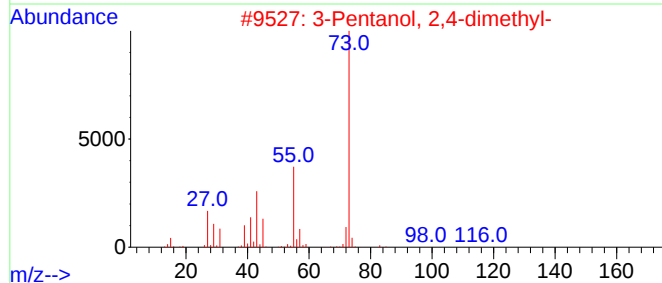
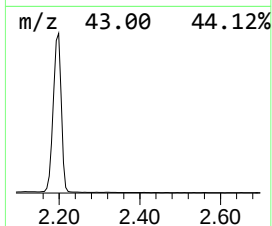
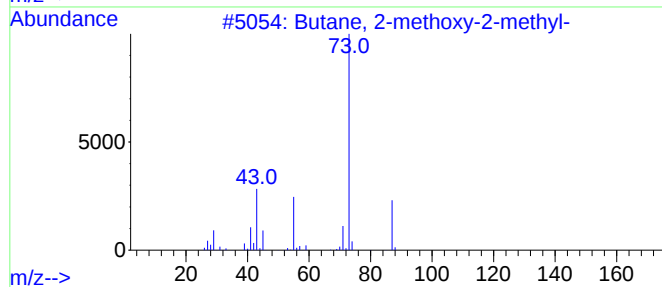
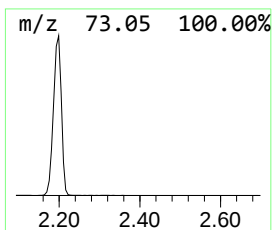
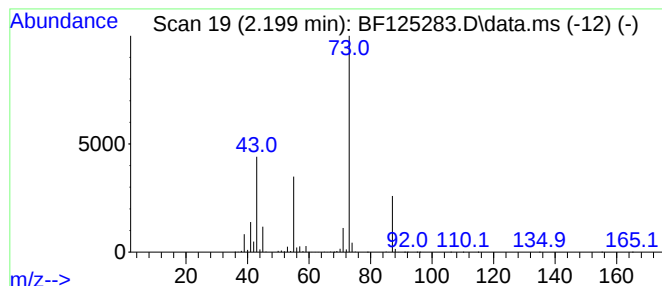
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.199	87.57 ng	5028440	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	39
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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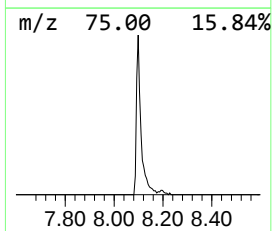
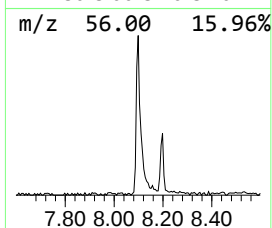
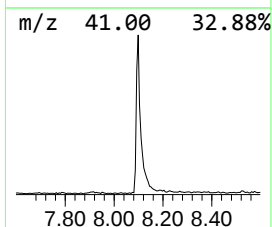
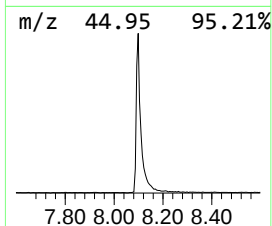
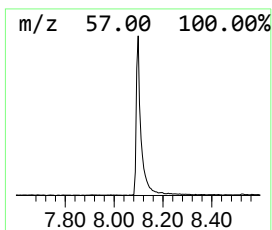
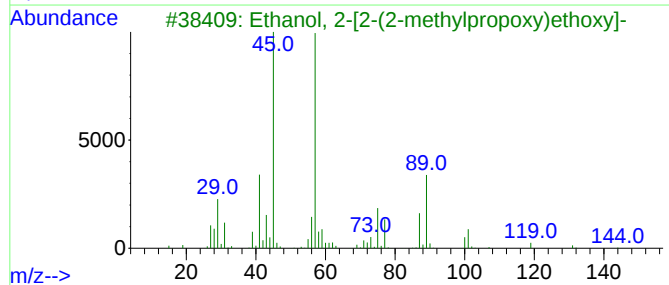
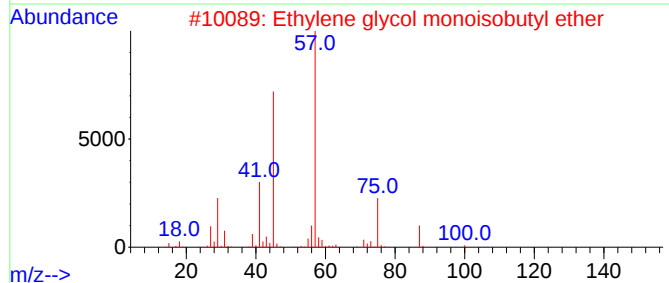
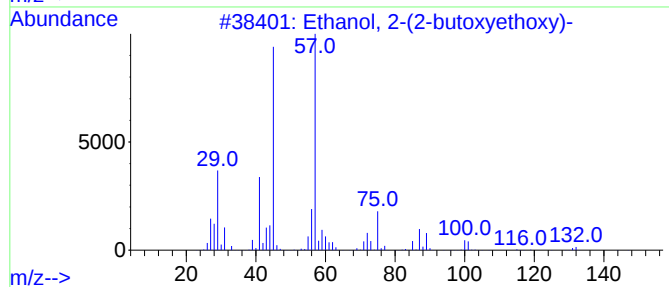
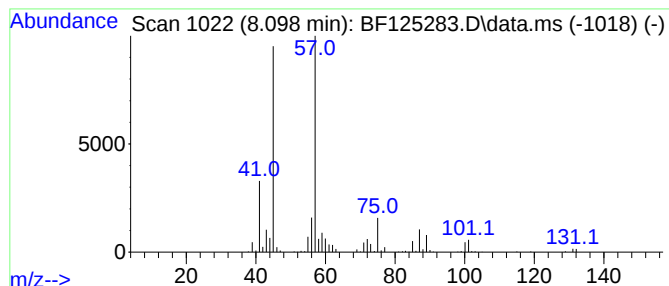
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	14.13 ng	1068540	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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47



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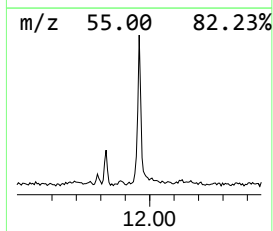
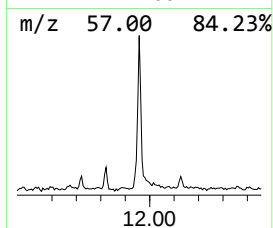
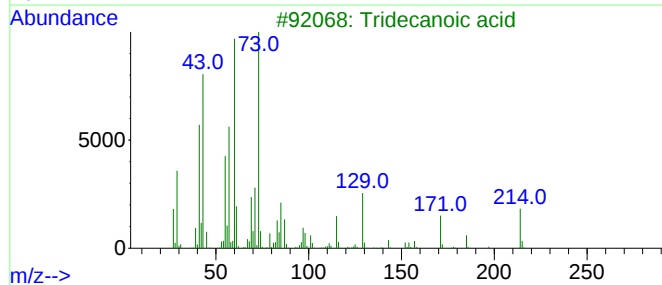
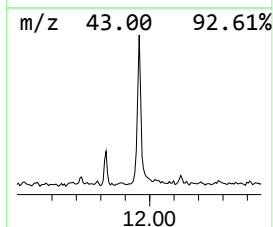
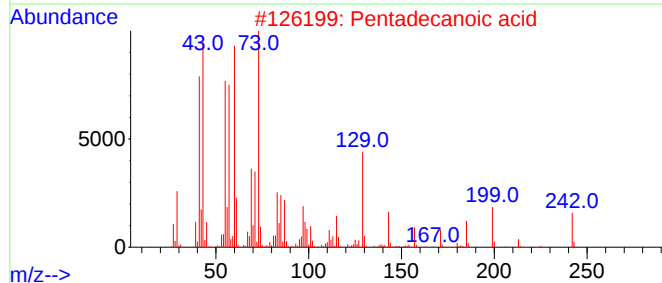
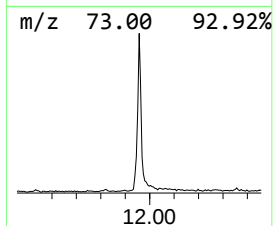
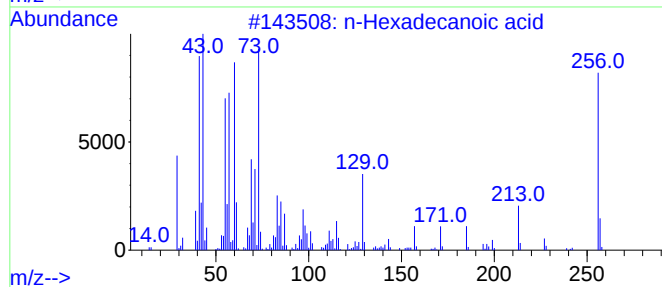
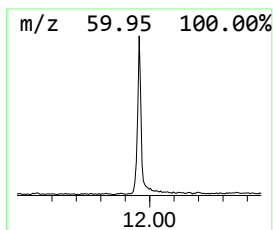
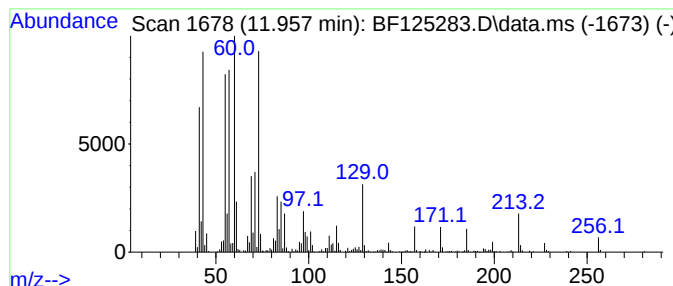
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	7.46 ng	745623	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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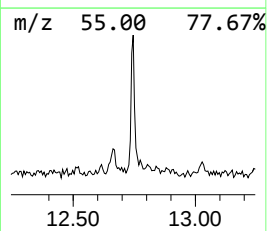
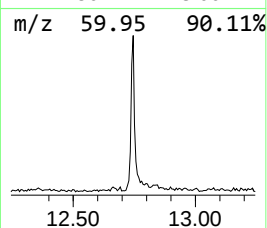
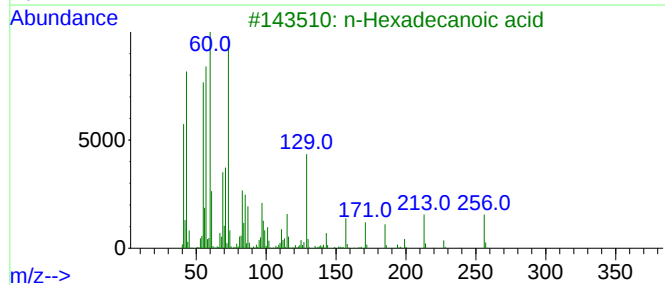
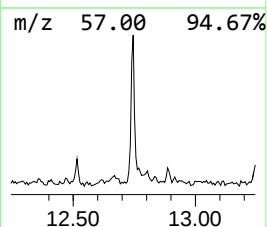
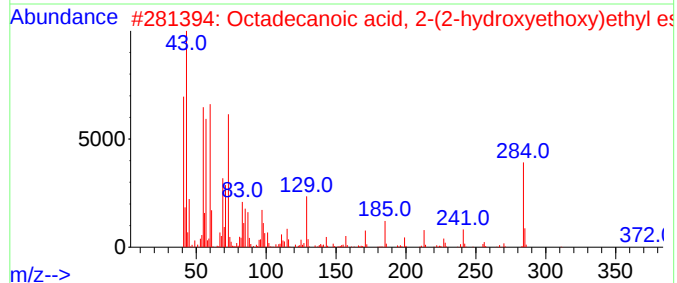
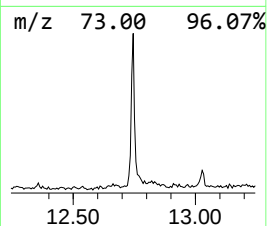
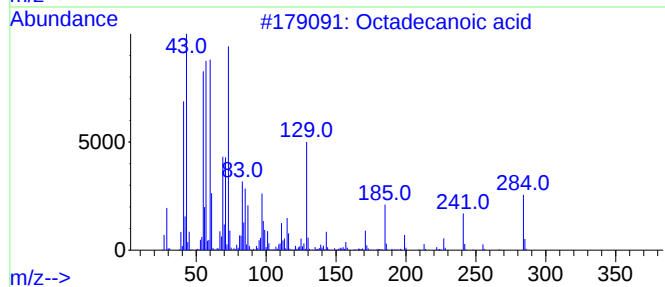
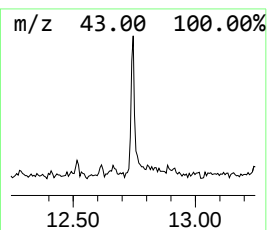
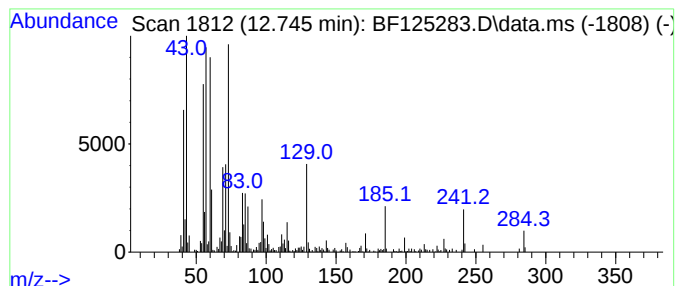
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.745	4.07 ng	407413	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	74



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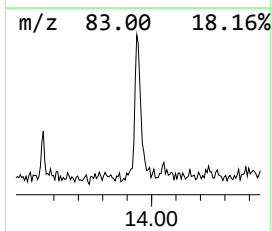
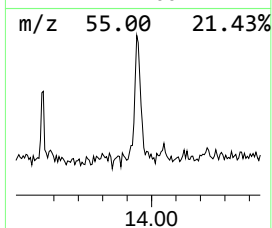
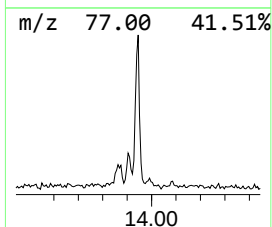
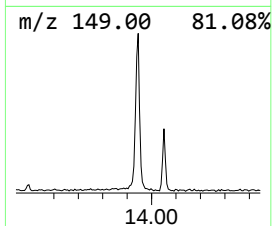
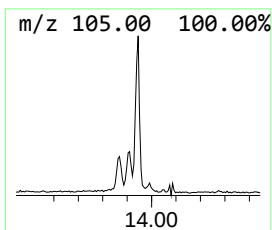
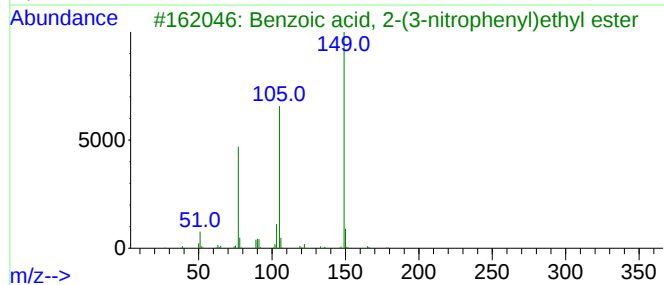
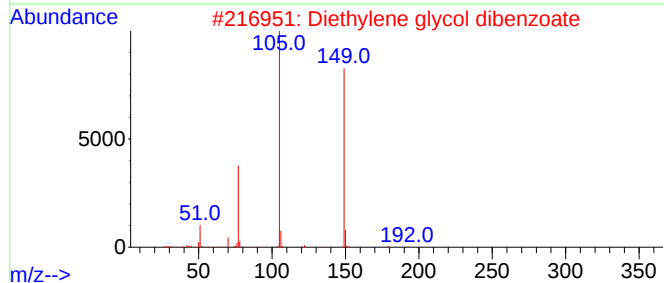
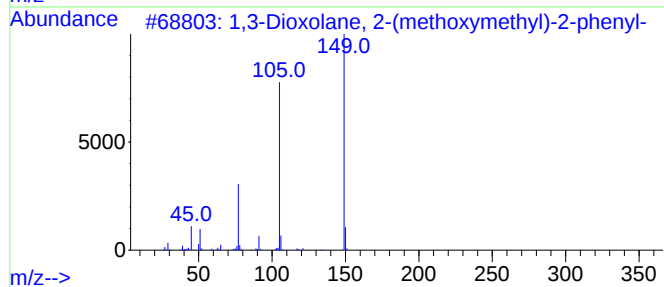
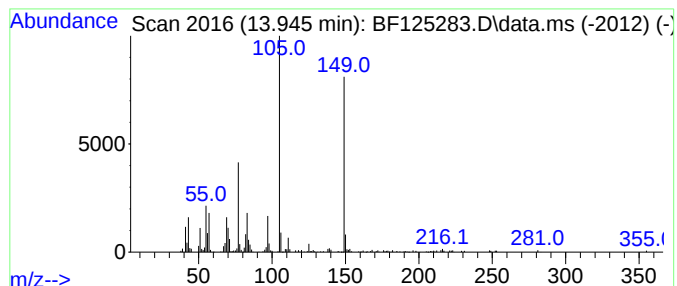
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Peak Number 5 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.945	3.82 ng	369076	Chrysene-d12		14.080	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...		194	C11H14O3	1000156-71-2	72
2	Diethylene glycol dibenzoate		314	C18H18O5	000120-55-8	72
3	Benzoic acid, 2-(3-nitrophenyl)e...		271	C15H13NO4	1000368-22-4	64
4	Phthalic acid, monodecyl ester		306	C18H26O4	024539-60-4	43
5	2,3-Dimethyl-4a,8a-diphenyl-hexa...		326	C20H22O4	1000297-07-0	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.199	87.6	ng	5028440	1	6.916	1148380	20.0
Ethanol, 2-(2-b...	8.098	14.1	ng	1068540	2	8.198	1512380	20.0
n-Hexadecanoic ...	11.957	7.5	ng	745623	4	11.439	1999770	20.0
Octadecanoic acid	12.745	4.1	ng	407413	4	11.439	1999770	20.0
1,3-Dioxolane, ...	13.945	3.8	ng	369076	5	14.080	1930610	20.0