

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
 Data File : BF139980.D
 Acq On : 23 Oct 2024 22:46
 Operator : RC/JU
 Sample : P4468-05
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ETGI-345

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139980.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	9	19	26	rVB	1924030	3129126	100.00%	12.363%
2	5.116	504	514	521	rVB	31422	52864	1.69%	0.209%
3	5.504	574	580	585	rBV	2076083	2727246	87.16%	10.776%
4	6.504	744	750	755	rBV	1999917	2699109	86.26%	10.664%
5	6.887	810	815	821	rVB	721367	929025	29.69%	3.671%
6	7.445	904	910	915	rBV	1373171	1769213	56.54%	6.990%
7	7.698	948	953	959	rBV	26110	31896	1.02%	0.126%
8	8.169	1027	1033	1038	rBV	942686	1161057	37.10%	4.587%
9	9.245	1210	1216	1226	rBV	2159775	2768865	88.49%	10.940%
10	9.922	1326	1331	1343	rVB	896061	1165442	37.24%	4.605%
11	10.634	1447	1452	1460	rBV	432341	555470	17.75%	2.195%
12	10.710	1460	1465	1477	rBV	1145729	1454088	46.47%	5.745%
13	10.945	1500	1505	1510	rVB	47104	57028	1.82%	0.225%
14	11.410	1579	1584	1591	rBV	798592	994134	31.77%	3.928%
15	11.933	1668	1673	1685	rBV	212611	337460	10.78%	1.333%
16	12.622	1786	1790	1802	rBV2	17521	37706	1.21%	0.149%
17	12.716	1802	1806	1815	rBV2	36802	70651	2.26%	0.279%
18	12.992	1848	1853	1859	rBV	1698649	2239930	71.58%	8.850%
19	13.816	1990	1993	2002	rVB	36728	53844	1.72%	0.213%
20	13.904	2002	2008	2016	rBV	81693	211943	6.77%	0.837%
21	14.051	2027	2033	2045	rVB	751089	1074917	34.35%	4.247%
22	14.398	2089	2092	2096	rBV	39437	53867	1.72%	0.213%
23	14.439	2096	2099	2103	rVB	31914	39566	1.26%	0.156%
24	14.651	2130	2135	2143	rVB	115325	171120	5.47%	0.676%
25	14.910	2174	2179	2187	rVB2	52963	91231	2.92%	0.360%
26	15.021	2194	2198	2204	rBV	56572	94537	3.02%	0.374%
27	15.086	2205	2209	2216	rVB3	27815	54461	1.74%	0.215%
28	15.174	2221	2224	2235	rVB	37308	65028	2.08%	0.257%
29	15.333	2244	2251	2257	rBV	92672	207299	6.62%	0.819%
30	15.527	2278	2284	2296	rVB	528763	862429	27.56%	3.408%
31	16.016	2363	2367	2373	rVB3	19793	38540	1.23%	0.152%
32	16.192	2392	2397	2404	rVB	58795	110414	3.53%	0.436%

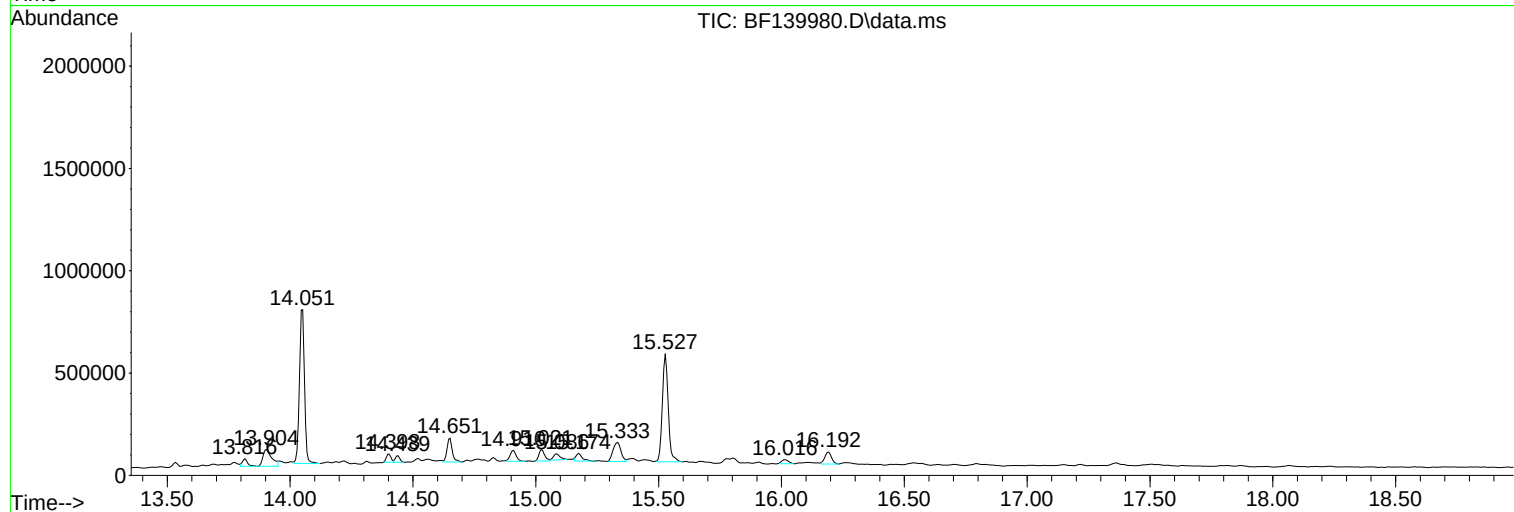
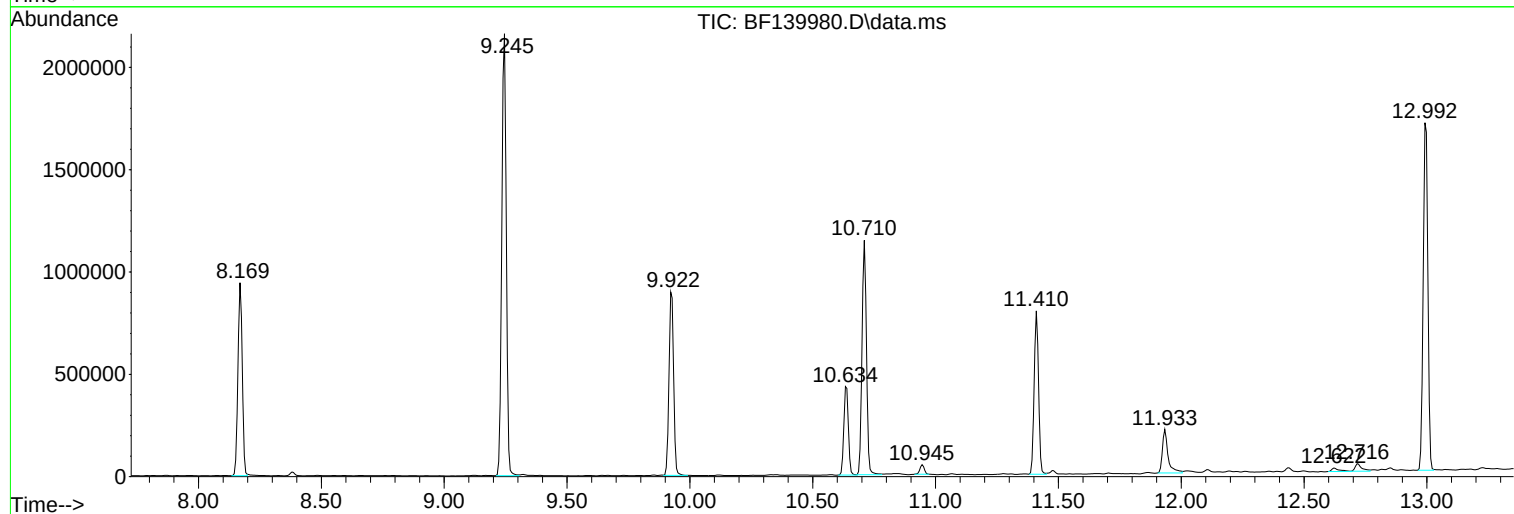
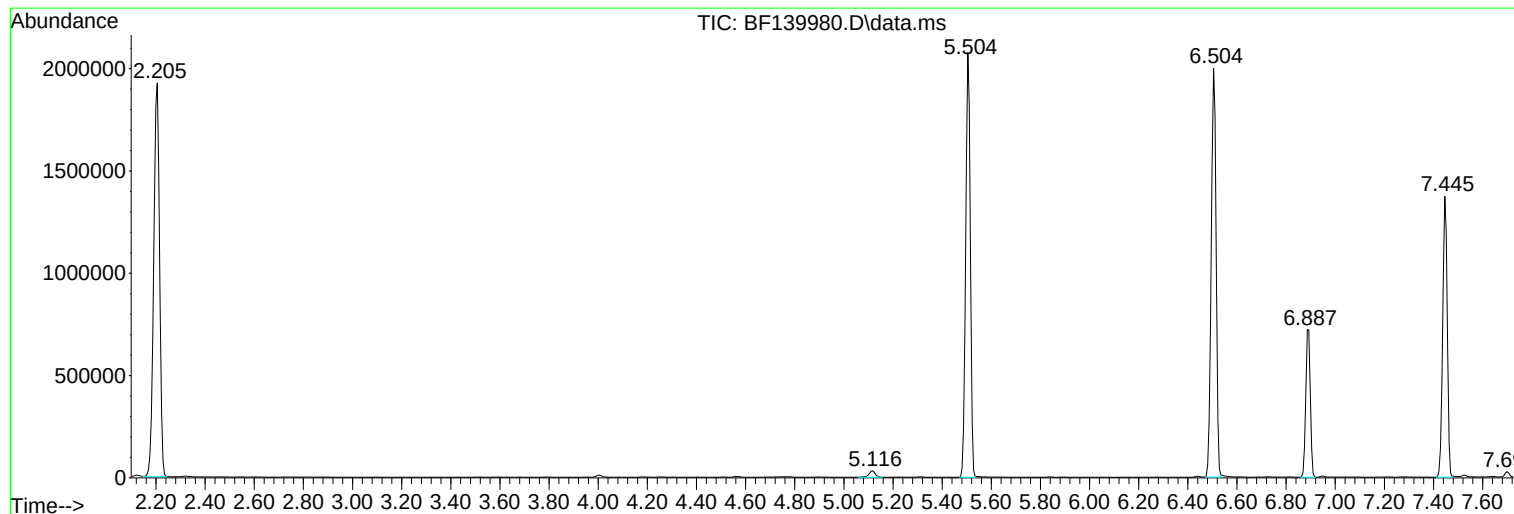
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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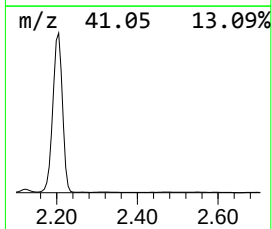
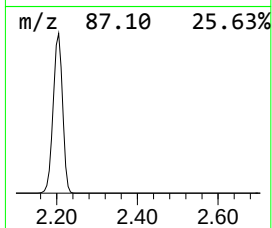
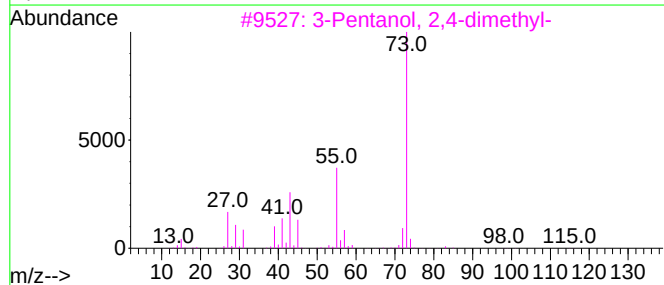
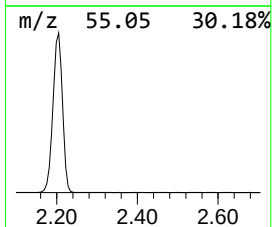
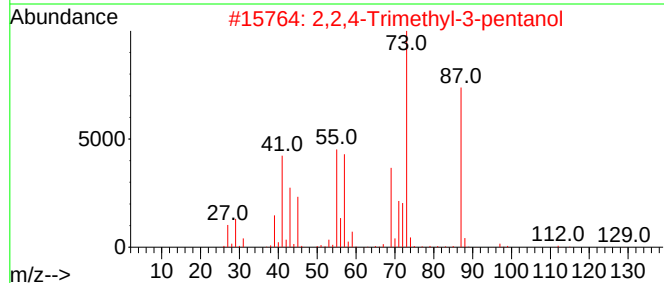
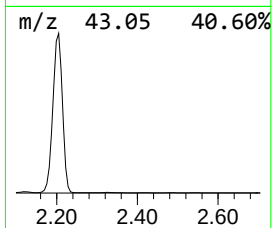
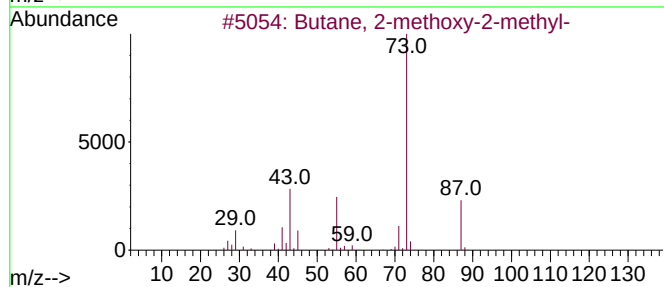
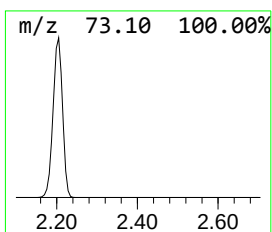
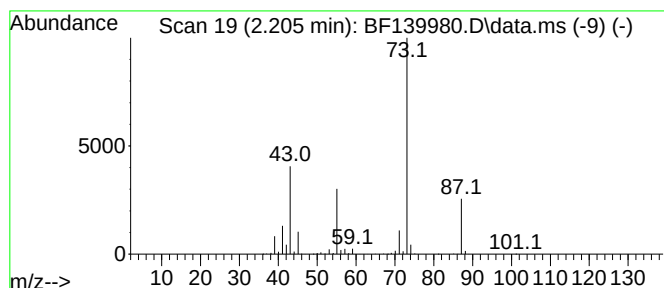
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	67.36 ng	3129130	1,4-Dichlorobenzene-d4	6.893

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	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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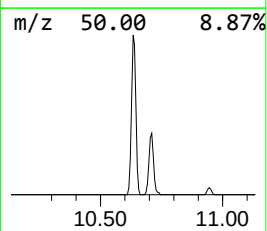
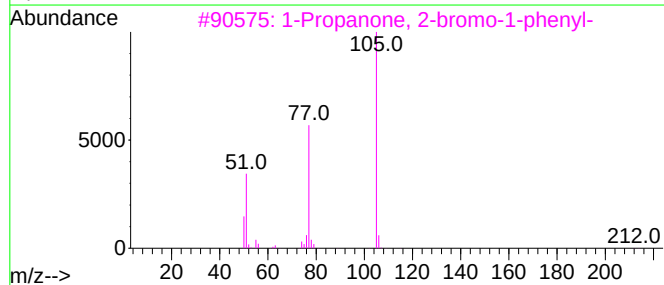
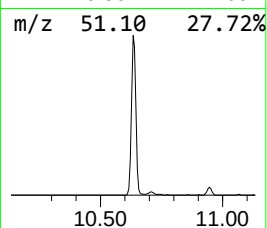
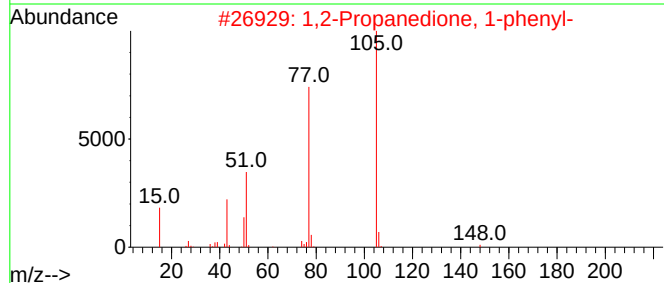
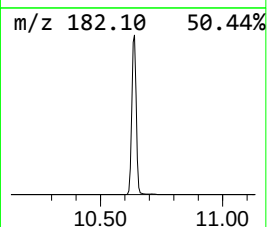
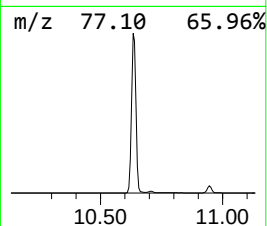
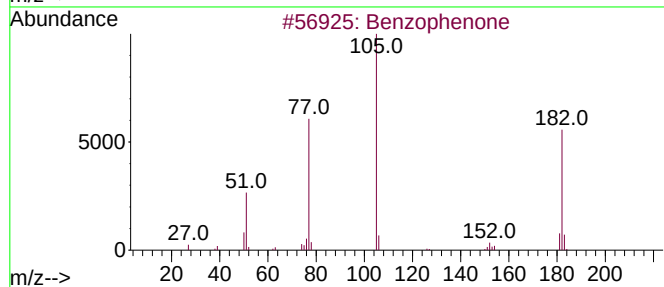
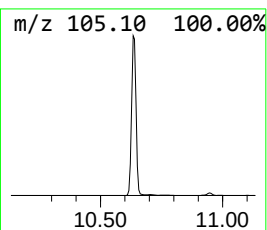
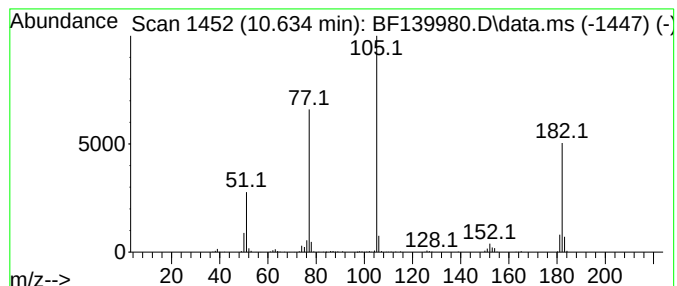
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	9.53 ng	555470	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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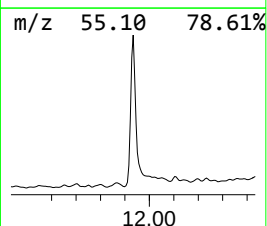
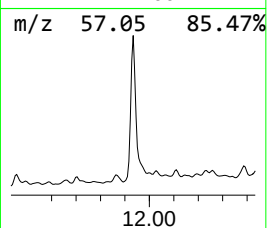
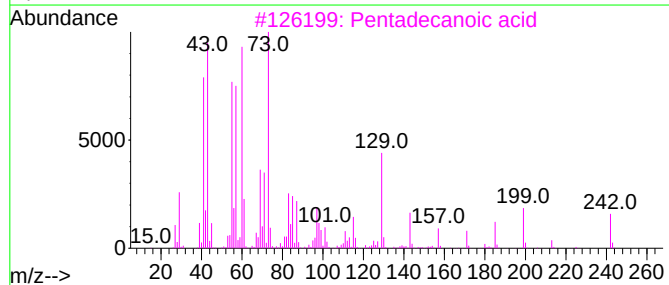
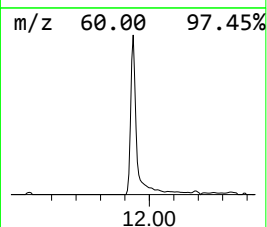
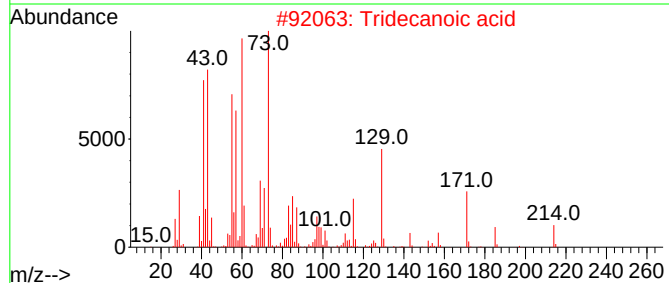
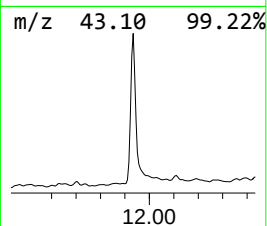
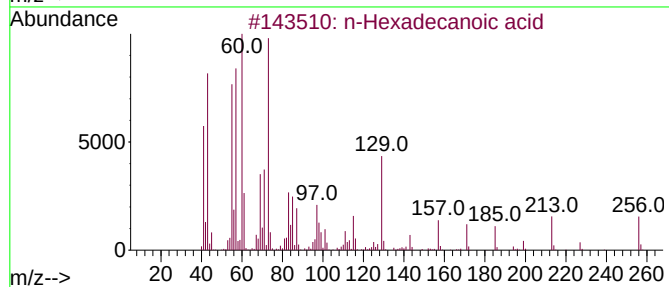
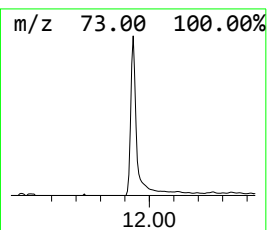
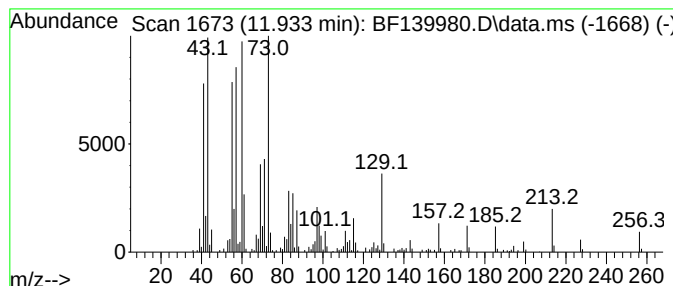
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	6.79 ng	337460	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Undecanoic acid	186	C11H22O2	000112-37-8	81
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78



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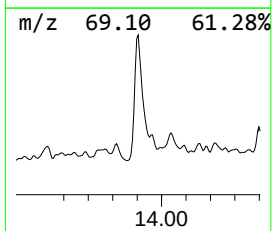
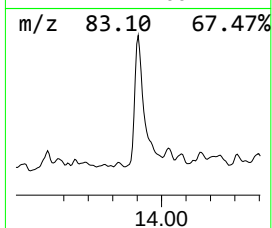
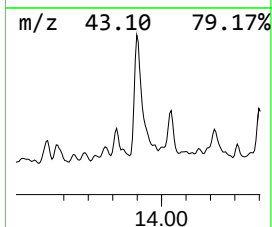
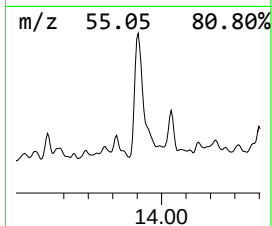
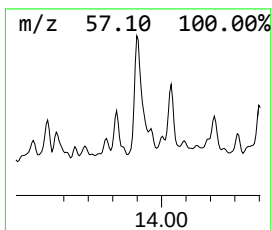
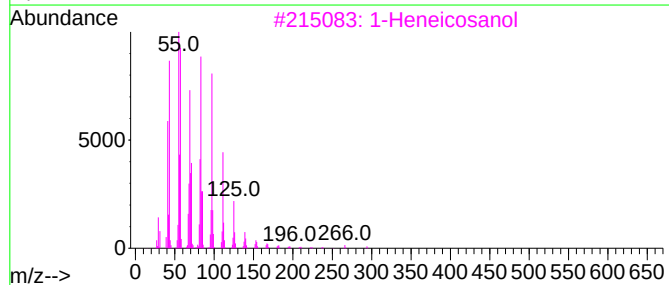
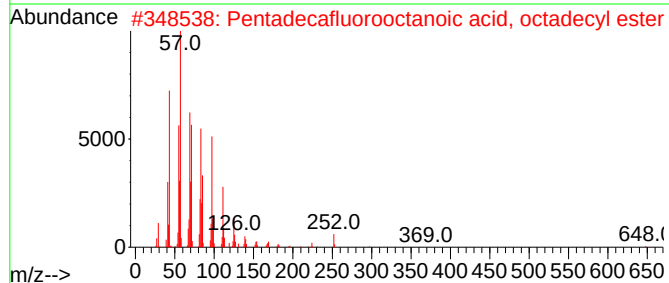
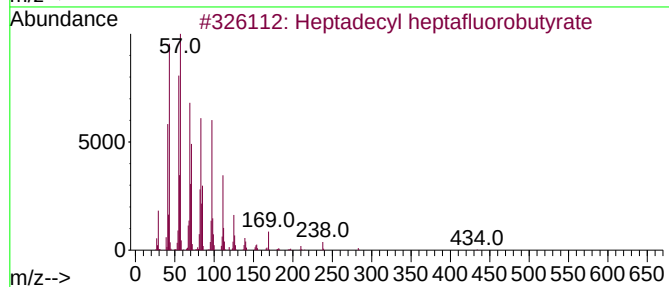
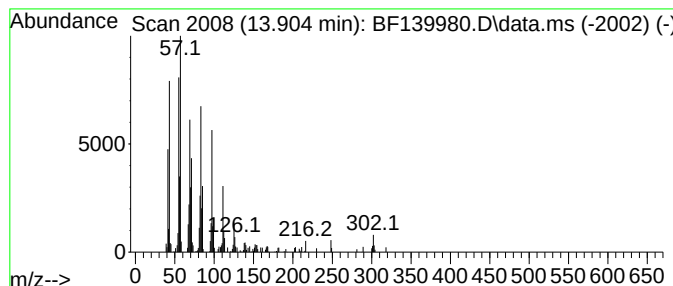
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.94 ng	211943	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



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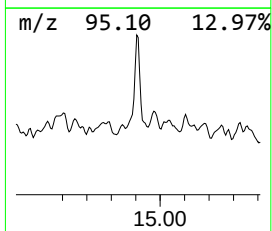
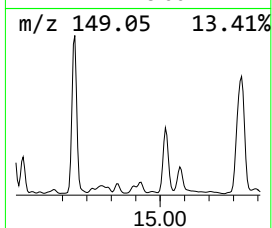
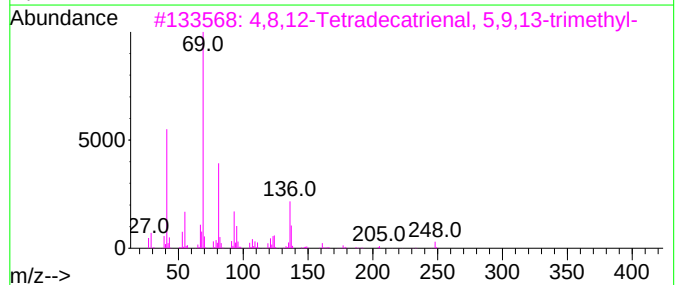
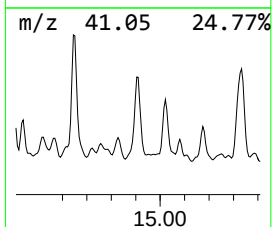
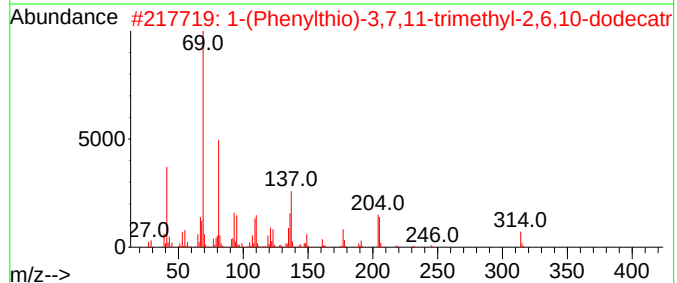
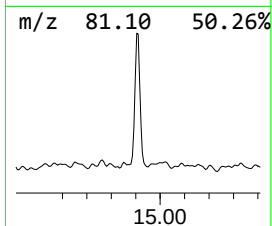
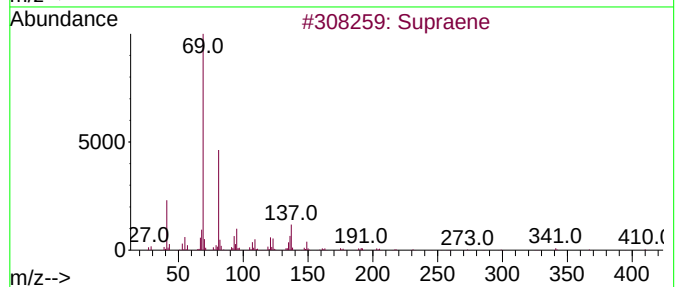
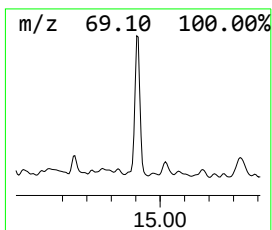
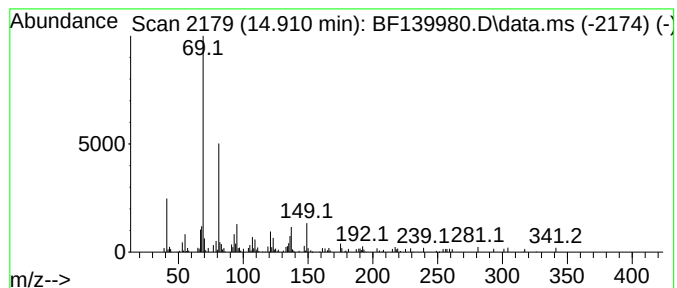
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Peak Number 5 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	2.12 ng	91231	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4			Umbelliprenin	366	C24H30O3	023838-17-7	59
5			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59



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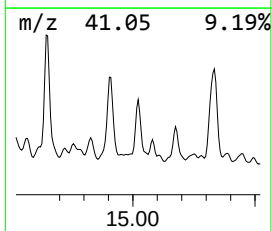
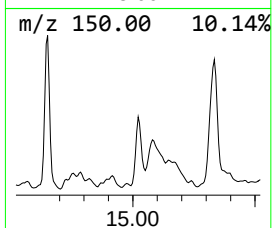
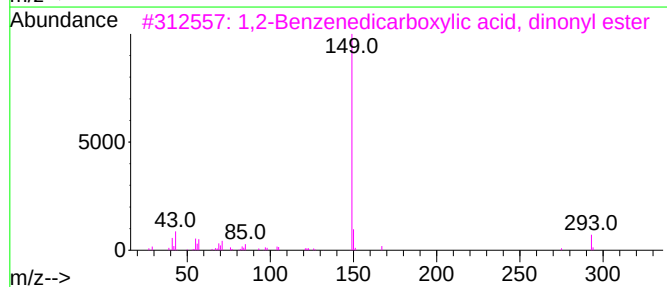
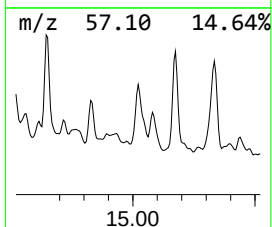
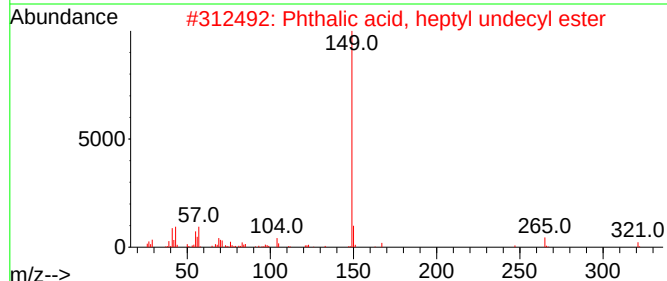
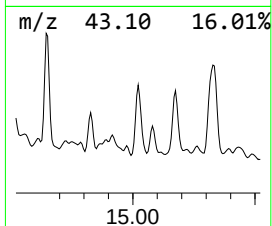
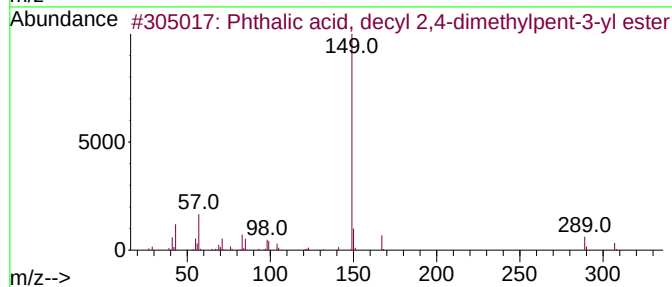
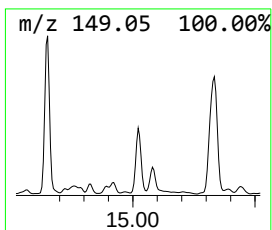
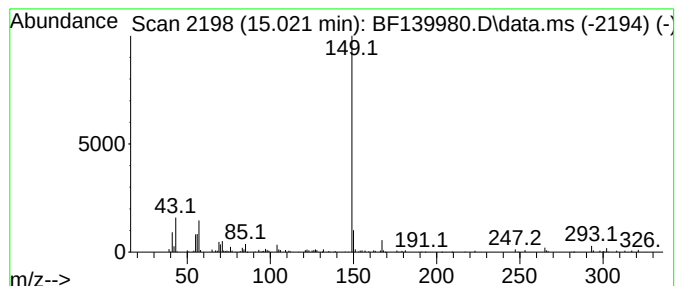
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phthalic acid, decyl 2,4-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.022	2.19 ng	94537	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, decyl 2,4-dimethy...	404	C25H40O4	1000356-84-9	86
2			Phthalic acid, heptyl undecyl ester	418	C26H42O4	1010308-94-0	80
3			1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	80
4			Phthalic acid, hexyl 4-methylhep...	362	C22H34O4	1000377-94-1	78
5			Phthalic acid, hex-3-yl isobutyl...	306	C18H26O4	1000356-95-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139980.D
Acq On : 23 Oct 2024 22:46
Operator : RC/JU
Sample : P4468-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

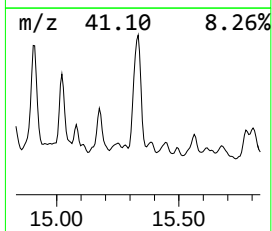
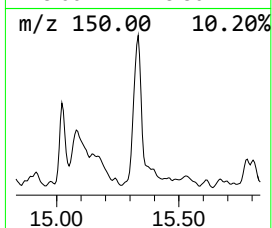
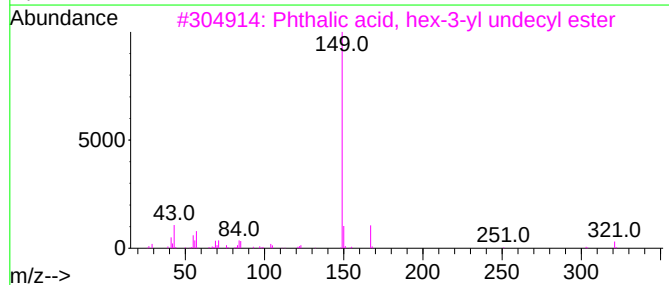
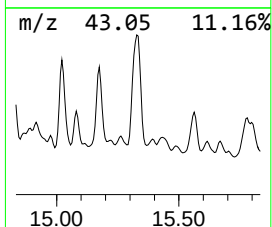
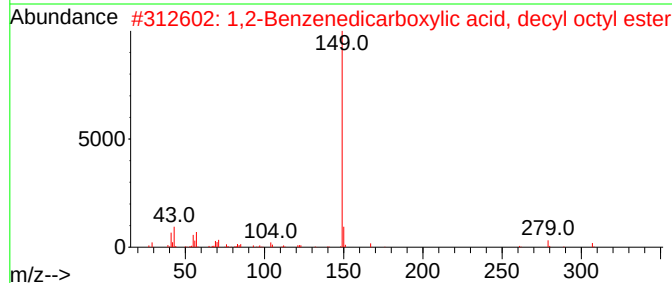
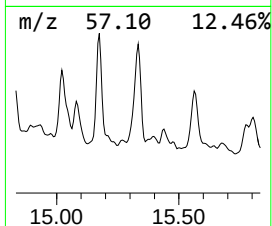
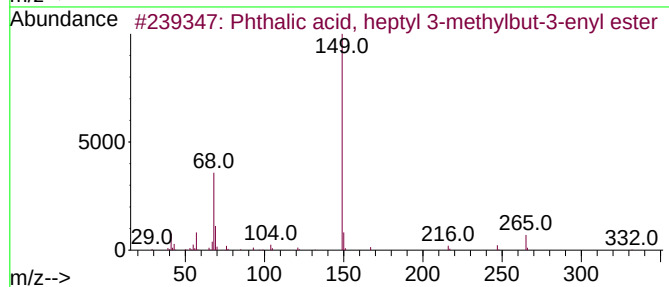
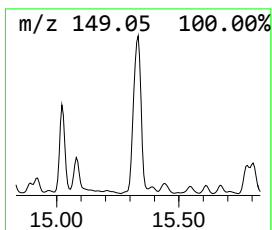
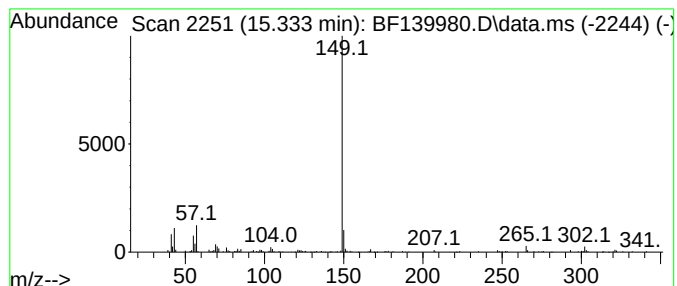
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phthalic acid, heptyl 3-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	4.81 ng	207299	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, heptyl 3-methylbu...	332	C20H28O4	1000357-10-5	83
2			1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	80
3			Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	80
4			1,2-Benzenedicarboxylic acid, di...	362	C22H34O4	003648-21-3	80
5			Phthalic acid, heptyl octyl ester	376	C23H36O4	088216-58-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139980.D
Acq On : 23 Oct 2024 22:46
Operator : RC/JU
Sample : P4468-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

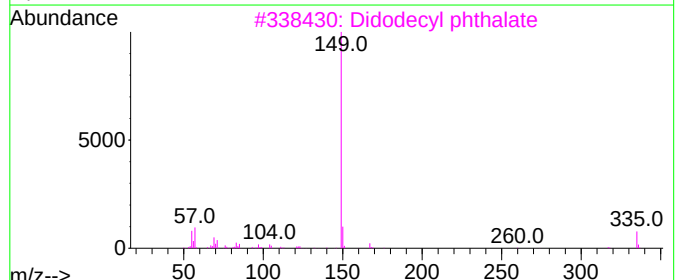
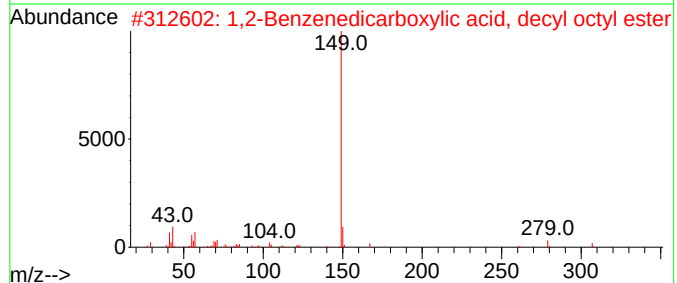
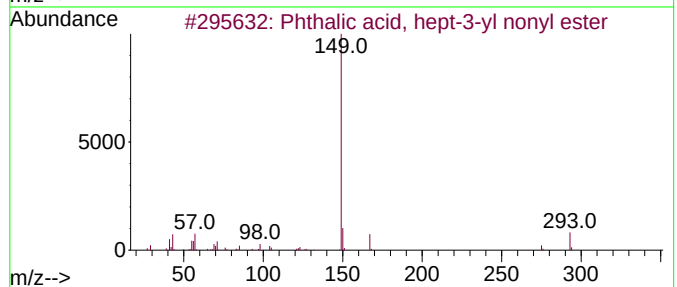
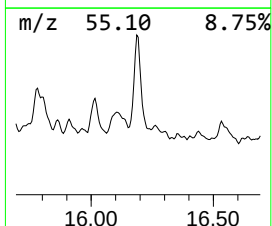
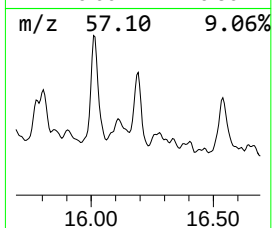
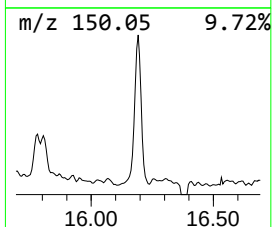
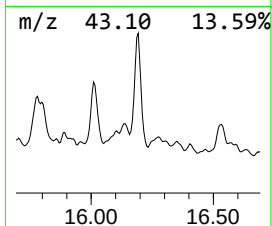
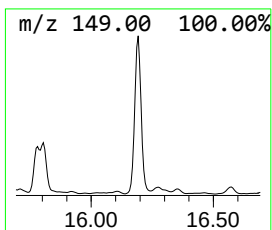
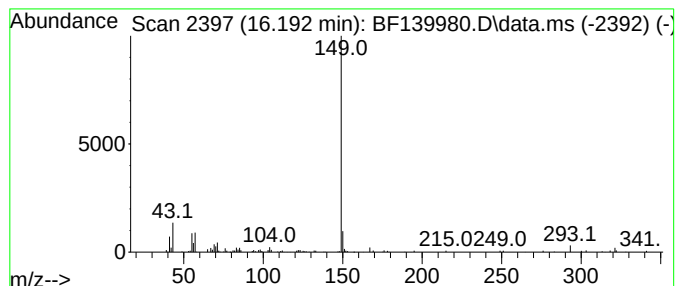
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phthalic acid, hept-3-yl no... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.192	2.56 ng	110414	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	80
2			1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	80
3			Didodecyl phthalate	502	C32H54O4	002432-90-8	80
4			Di-n-octyl phthalate	390	C24H38O4	000117-84-0	80
5			1,2-Benzenedicarboxylic acid, di...	418	C26H42O4	000084-76-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139980.D
Acq On : 23 Oct 2024 22:46
Operator : RC/JU
Sample : P4468-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-345

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	2.205	67.4	ng	3129130	1	6.893	929025	20.0
Benzophenone	10.634	9.5	ng	555470	3	9.922	1165440	20.0
n-Hexadecanoic ...	11.933	6.8	ng	337460	4	11.410	994134	20.0
Heptadecyl hept...	13.904	3.9	ng	211943	5	14.051	1074920	20.0
Supraene	14.910	2.1	ng	91231	6	15.527	862429	20.0
Phthalic acid, ...	15.022	2.2	ng	94537	6	15.527	862429	20.0
Phthalic acid, ...	15.333	4.8	ng	207299	6	15.527	862429	20.0
Phthalic acid, ...	16.192	2.6	ng	110414	6	15.527	862429	20.0