

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
 Data File : BF133271.D
 Acq On : 05 May 2023 19:17
 Operator : CG\JU
 Sample : 02618-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DSN003

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.910	476	480	489	rVB	385674	422911	7.07%	1.137%
2	5.346	548	554	558	rVB	1538762	2688089	44.96%	7.230%
3	6.363	723	727	730	rBV	1927024	1562147	26.13%	4.201%
4	6.722	785	788	793	rBV	1418822	1126444	18.84%	3.030%
5	7.292	879	885	888	rBV	3708889	3682135	61.59%	9.903%
6	8.010	1003	1007	1010	rBV	1860857	1524067	25.49%	4.099%
7	8.357	1063	1066	1072	rBV2	55359	94044	1.57%	0.253%
8	9.087	1185	1190	1193	rBV	6226707	5978823	100.00%	16.080%
9	9.757	1301	1304	1308	rVB	2001563	1657917	27.73%	4.459%
10	10.475	1422	1426	1430	rBV	1298062	1012588	16.94%	2.723%
11	10.551	1434	1439	1442	rBV	3798488	3724007	62.29%	10.016%
12	10.616	1448	1450	1454	rVB	112815	97606	1.63%	0.263%
13	10.781	1474	1478	1481	rVB	231786	209502	3.50%	0.563%
14	11.004	1512	1516	1519	rBV	555939	441801	7.39%	1.188%
15	11.110	1530	1534	1542	rVB3	50823	61960	1.04%	0.167%
16	11.239	1553	1556	1560	rVB	2079686	1724889	28.85%	4.639%
17	11.416	1582	1586	1592	rVB2	146869	163895	2.74%	0.441%
18	11.780	1644	1648	1651	rBV	481826	496882	8.31%	1.336%
19	12.563	1777	1781	1793	rBV2	95058	137756	2.30%	0.370%
20	12.751	1810	1813	1817	rVB	81280	70443	1.18%	0.189%
21	12.833	1821	1827	1830	rBV	5618713	5910253	98.85%	15.896%
22	13.204	1888	1890	1893	rBV	90512	80729	1.35%	0.217%
23	13.733	1977	1980	1994	rVB	185874	309323	5.17%	0.832%
24	13.874	1999	2004	2007	rBV	1657787	1518140	25.39%	4.083%
25	13.969	2014	2020	2031	rBV	890852	980770	16.40%	2.638%
26	14.721	2144	2148	2153	rVB	167440	162005	2.71%	0.436%
27	15.292	2240	2245	2249	rBV	1095408	1276223	21.35%	3.432%
28	15.333	2249	2252	2259	rVB2	48425	66450	1.11%	0.179%

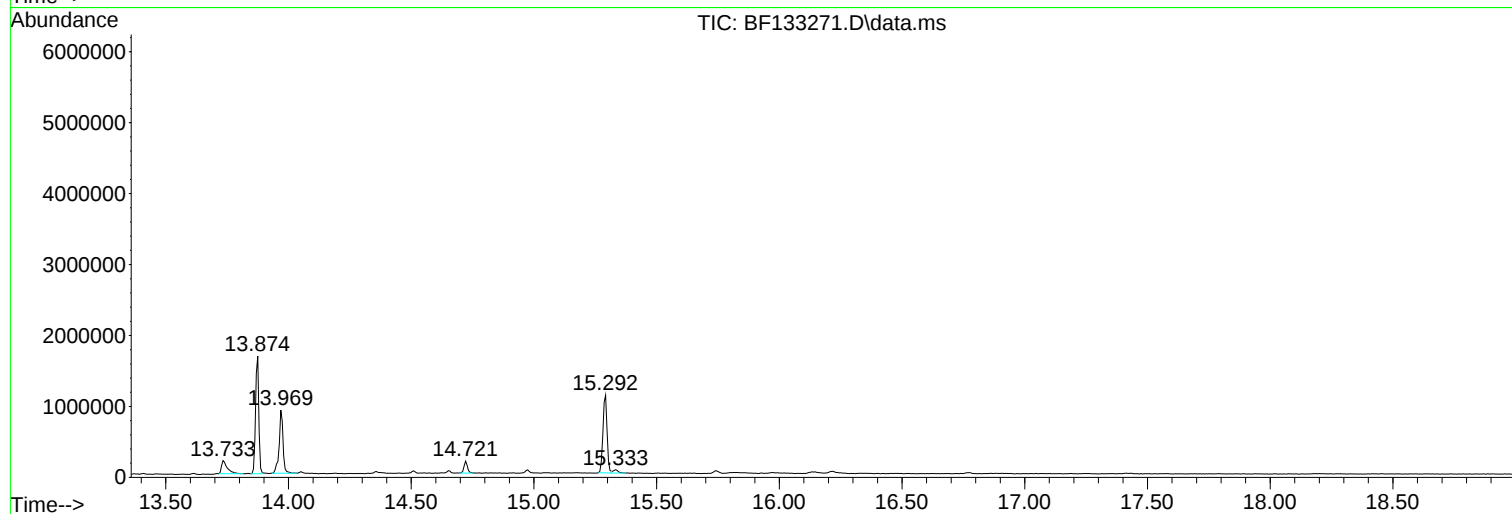
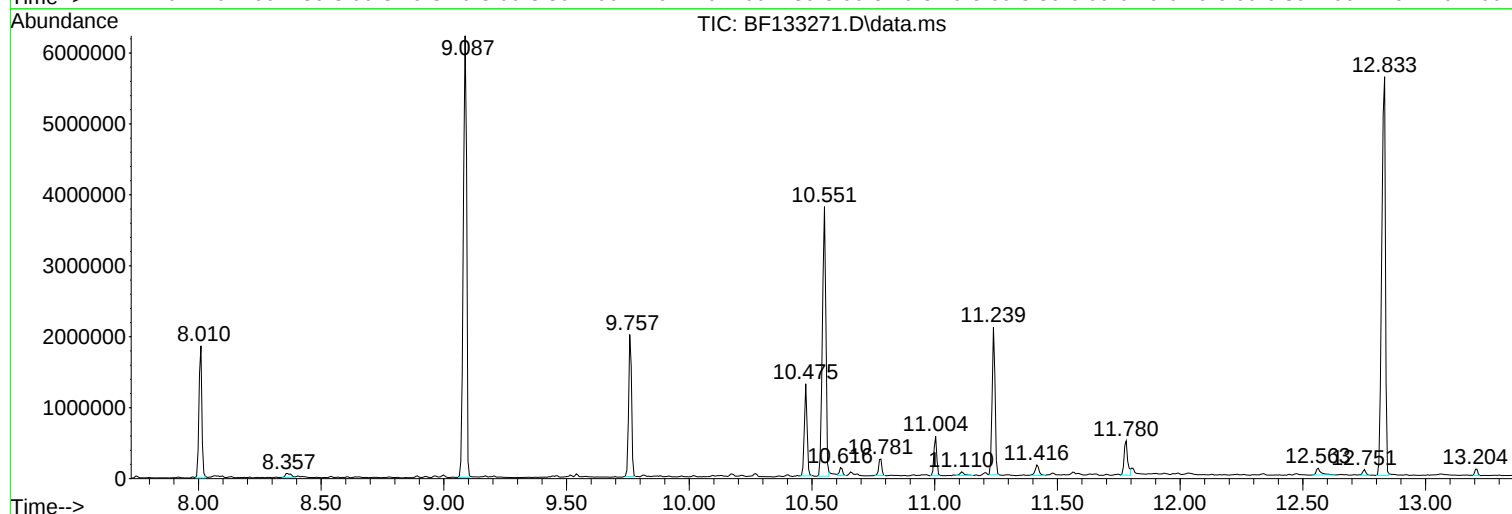
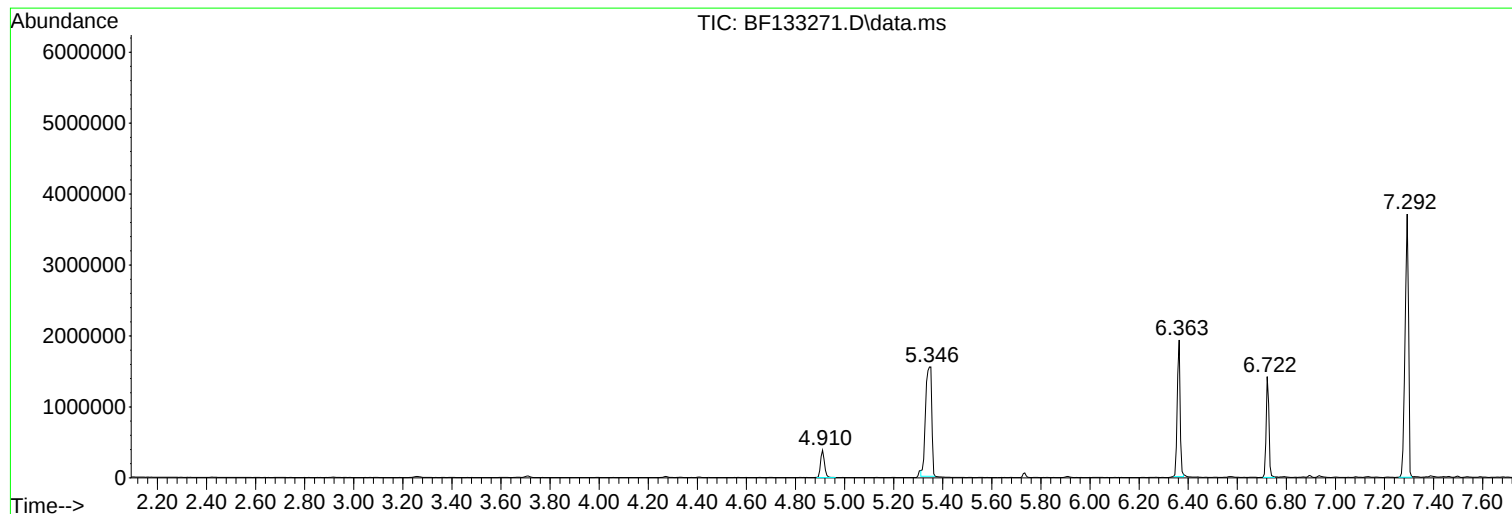
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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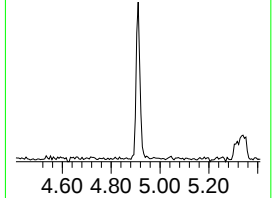
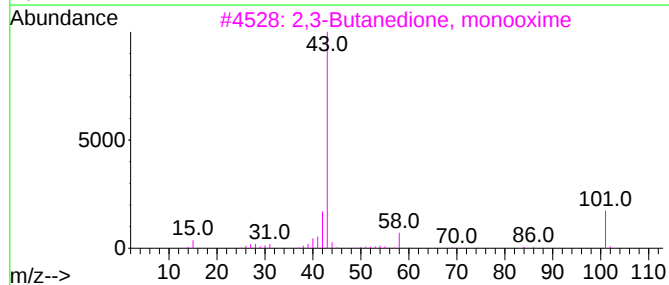
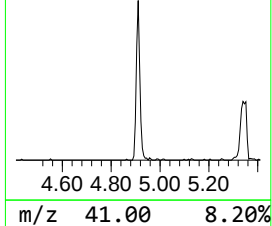
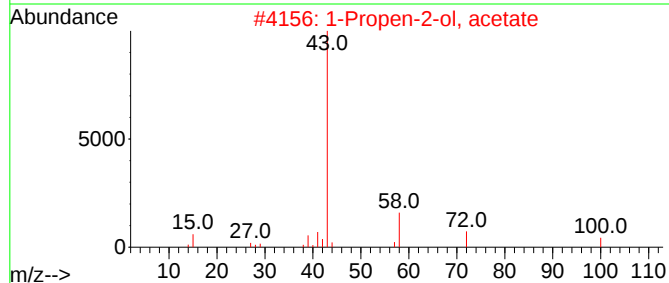
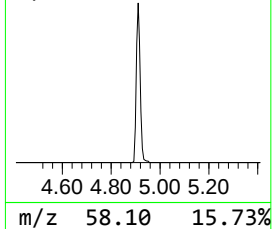
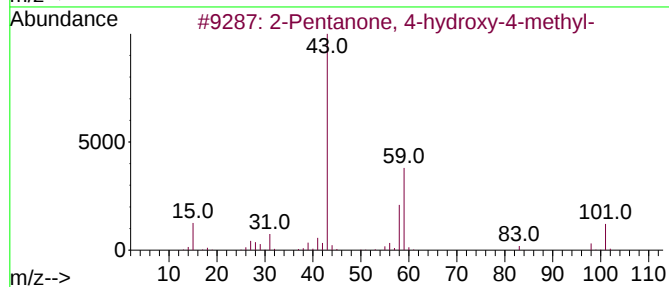
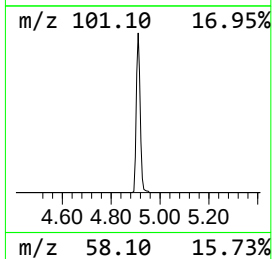
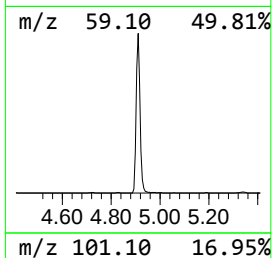
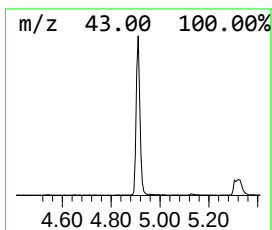
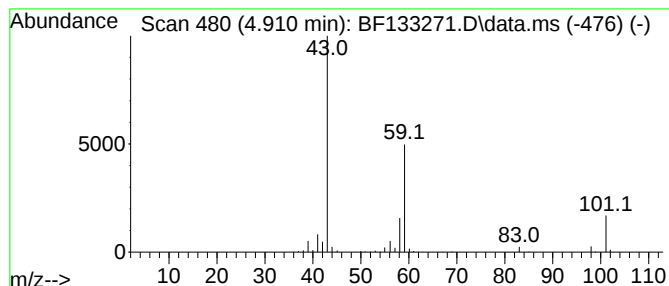
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	7.51 ng	422911	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9		



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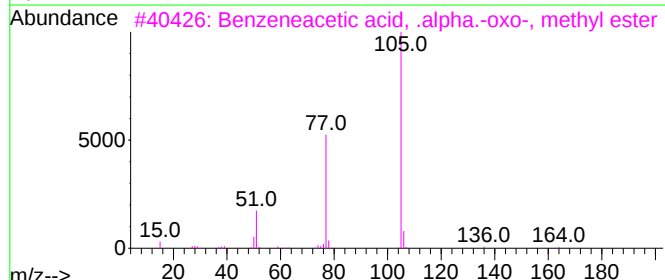
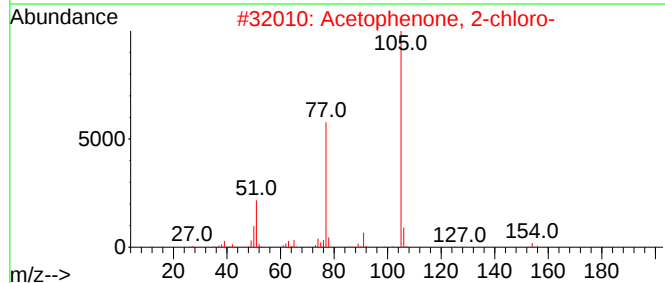
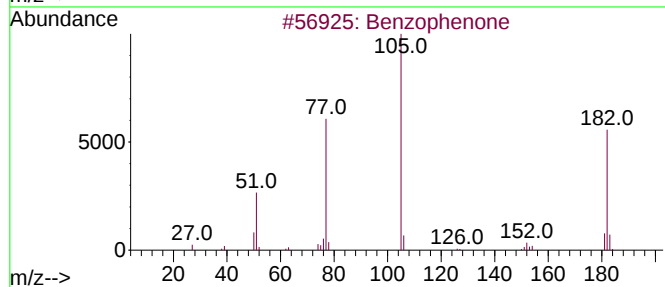
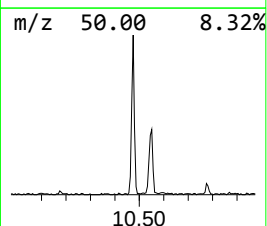
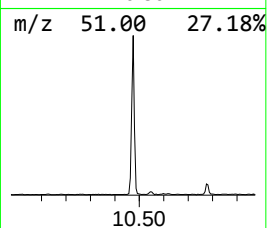
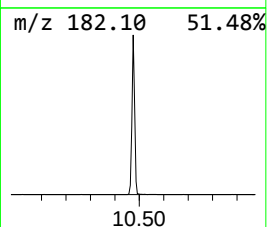
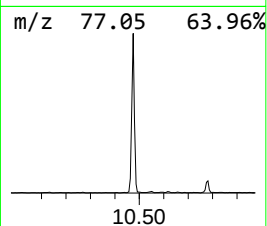
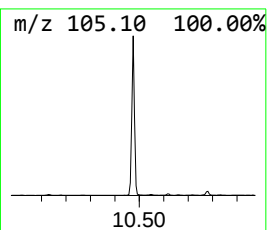
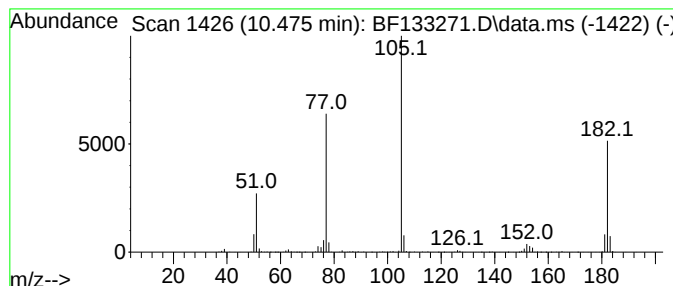
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	12.22 ng	1012590	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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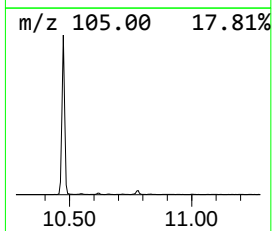
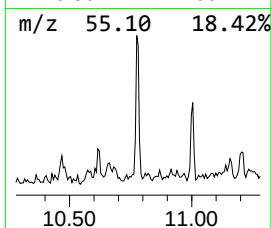
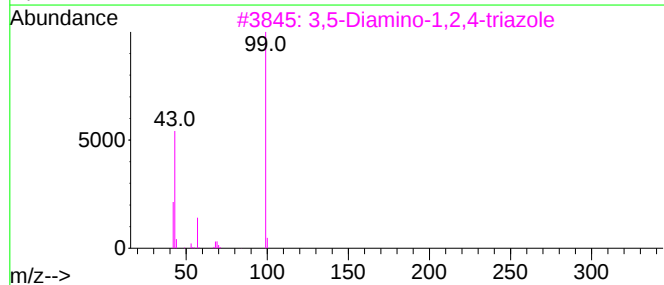
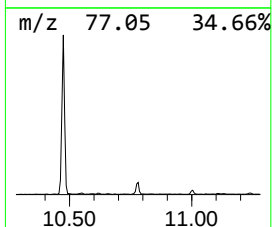
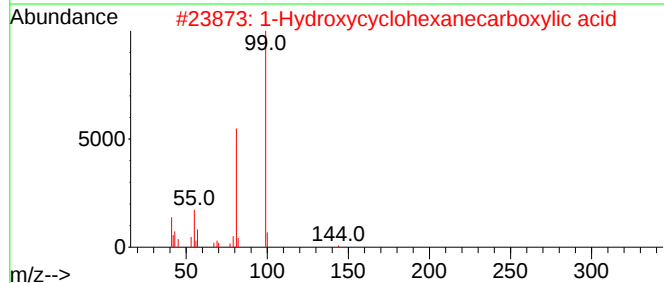
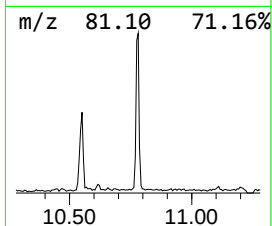
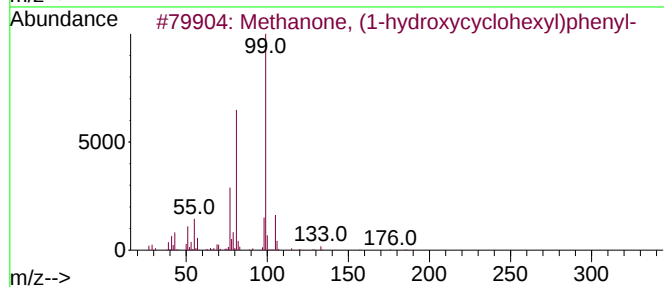
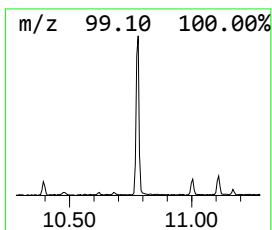
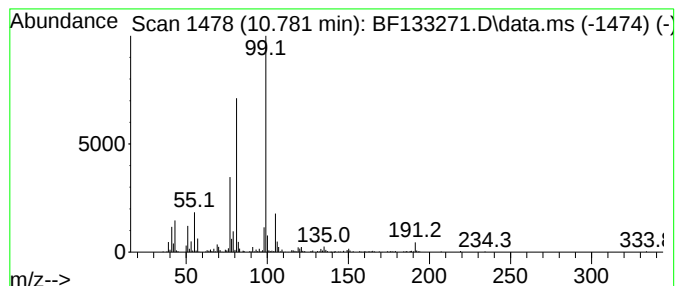
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Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	2.43 ng	209502	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	47
3			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	43
4			Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	38
5			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	38



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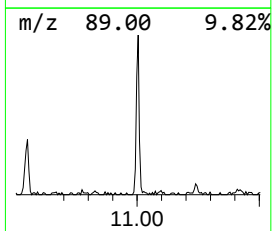
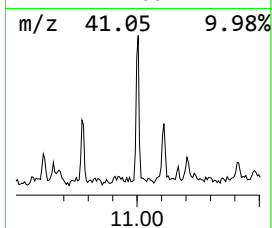
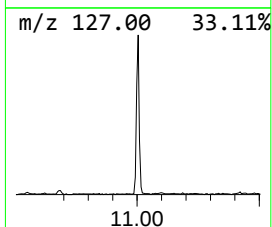
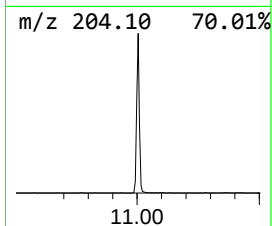
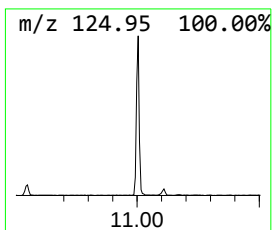
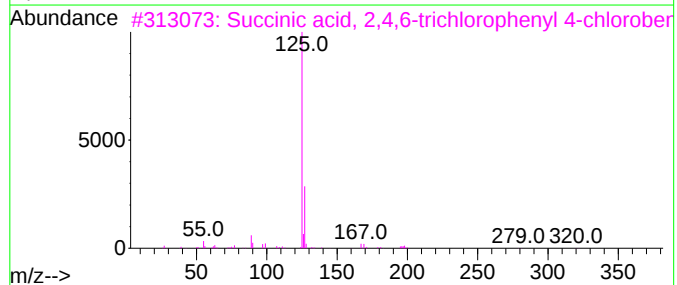
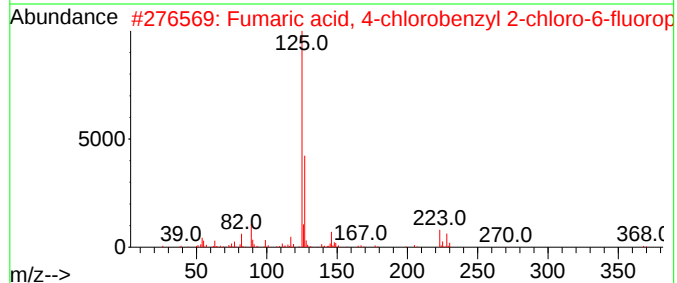
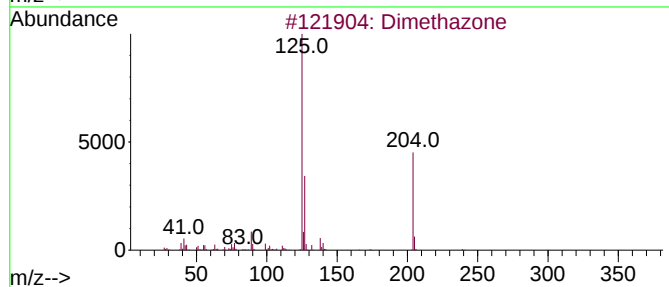
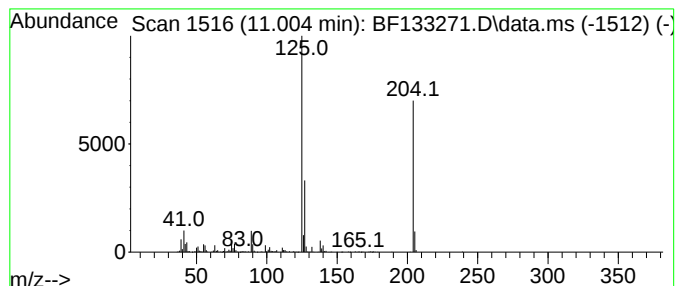
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Peak Number 4 Dimethazone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.004	5.12 ng	441801	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethazone	239	C12H14ClNO2	081777-89-1	80
2			Fumaric acid, 4-chlorobenzyl 2-c...	368	C17H11Cl12F04	1000405-92-1	50
3			Succinic acid, 2,4,6-trichloroph...	420	C17H12Cl4O4	1010389-68-3	50
4			4-(4-Chlorobenzyl)-4H-1,2,4-tria...	225	C9H8ClN3S	1000488-30-7	50
5			N-{3,5-Dichloro-4-[(4-chlorobenz...	383	C19H20Cl13NO	1010482-45-0	50



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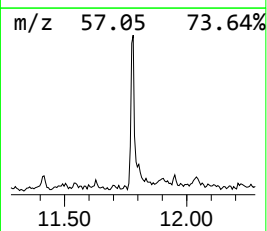
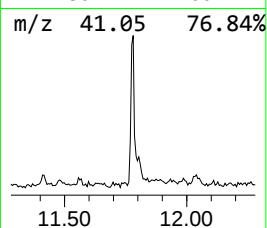
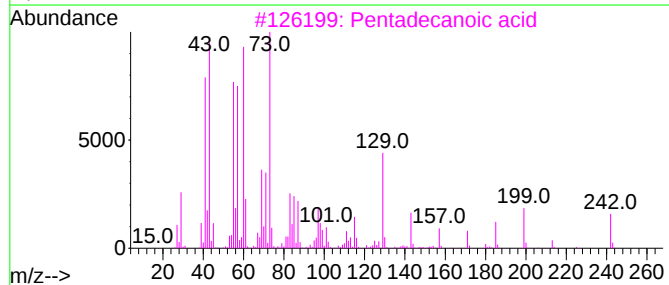
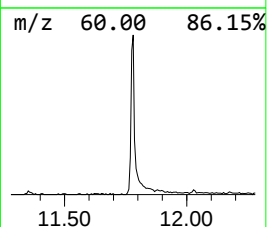
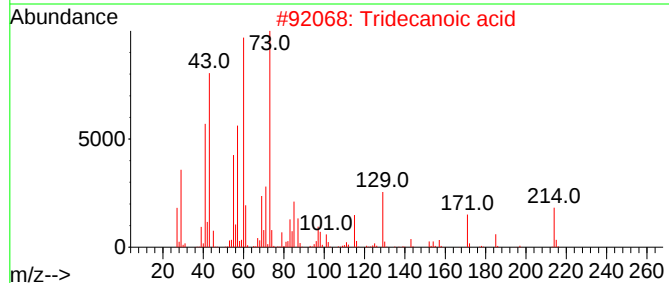
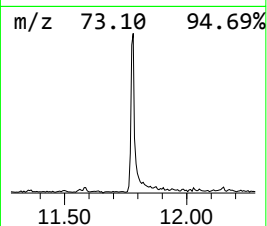
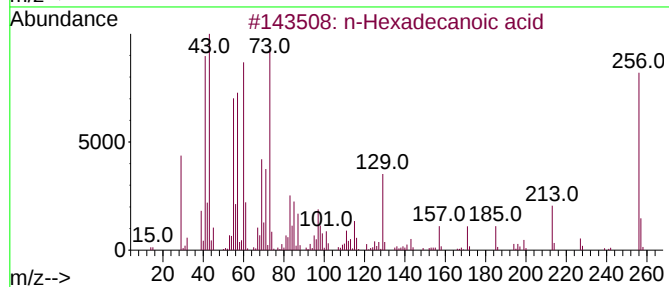
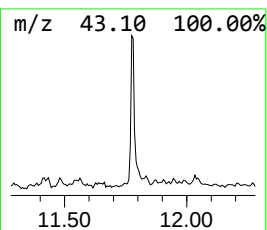
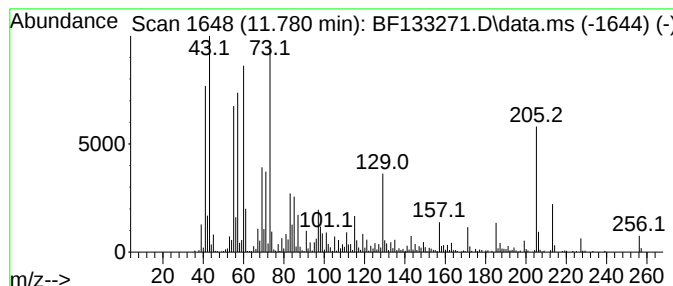
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	5.76 ng	496882	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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DSN003

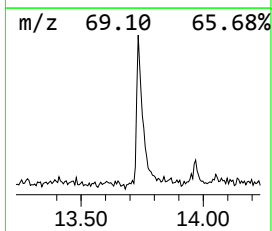
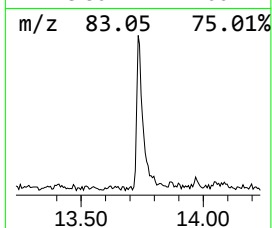
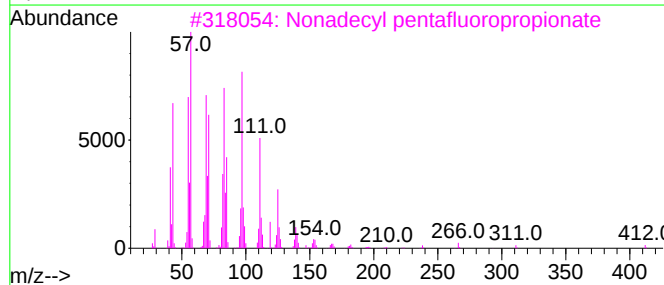
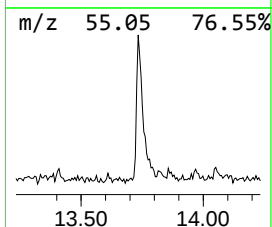
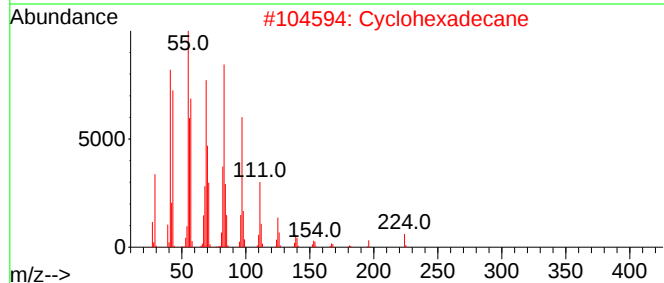
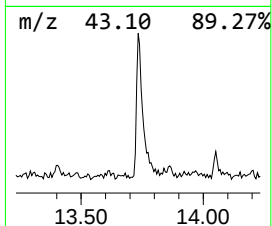
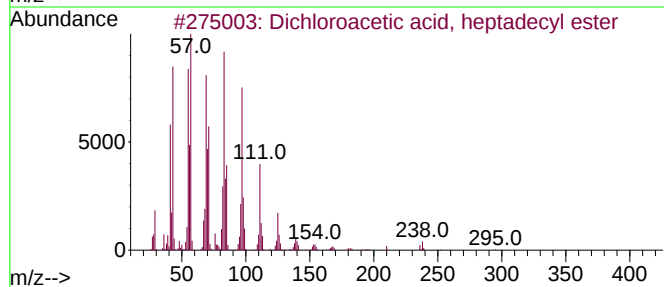
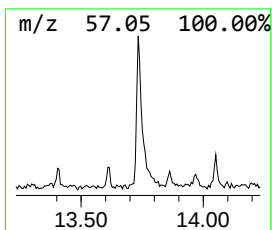
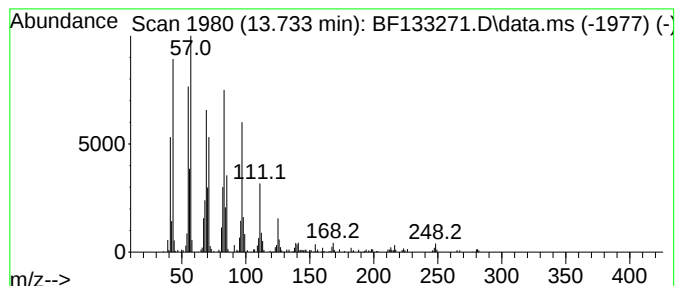
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	4.08 ng	309323	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			Cyclohexadecane	224	C16H32	000295-65-8	93
3			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133271.D
Acq On : 05 May 2023 19:17
Operator : CG\JU
Sample : 02618-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

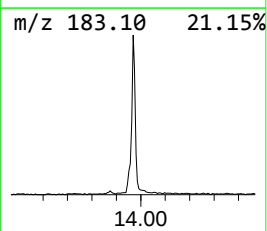
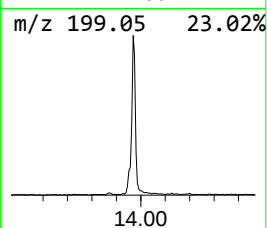
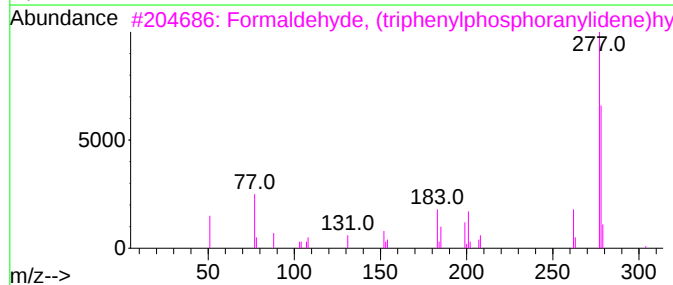
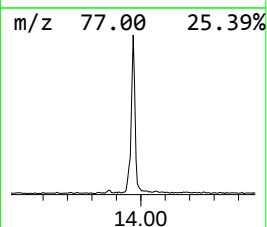
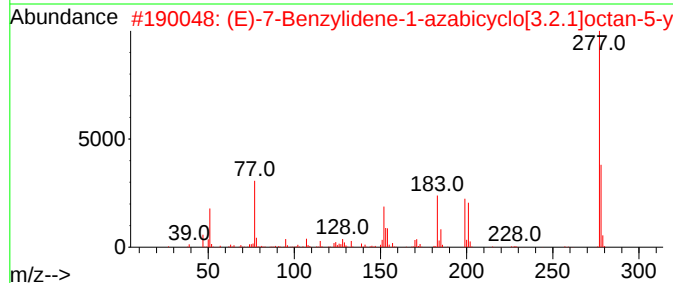
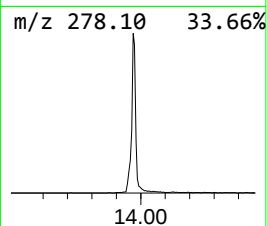
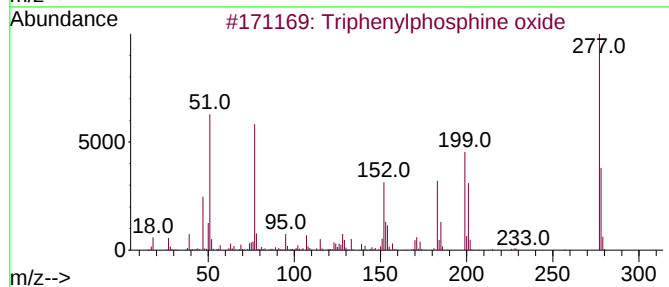
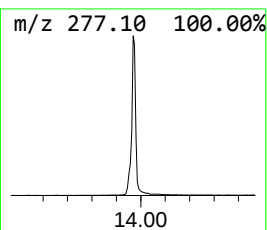
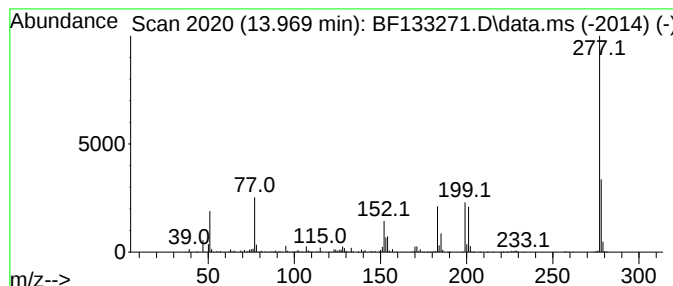
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	12.92 ng	980770	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	87
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133271.D
Acq On : 05 May 2023 19:17
Operator : CG\JU
Sample : 02618-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

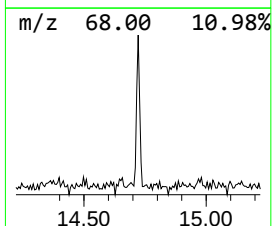
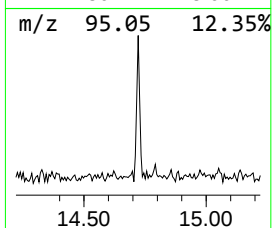
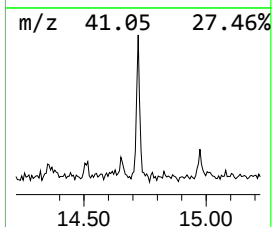
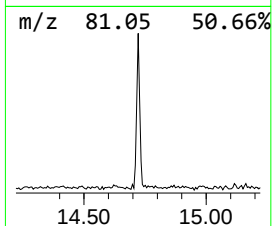
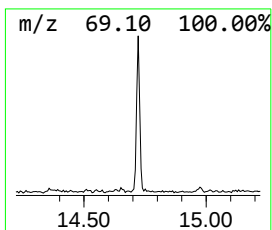
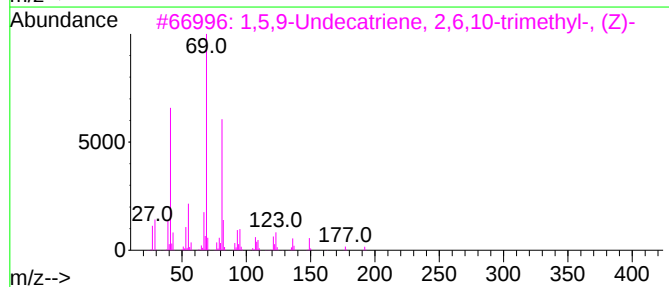
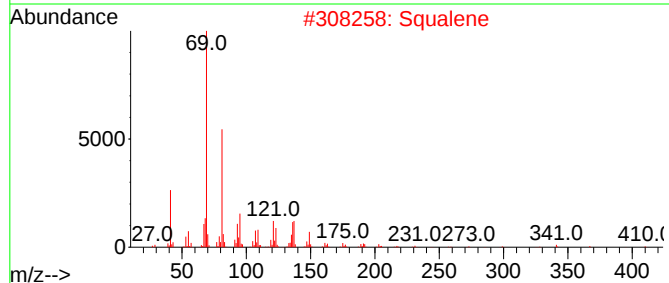
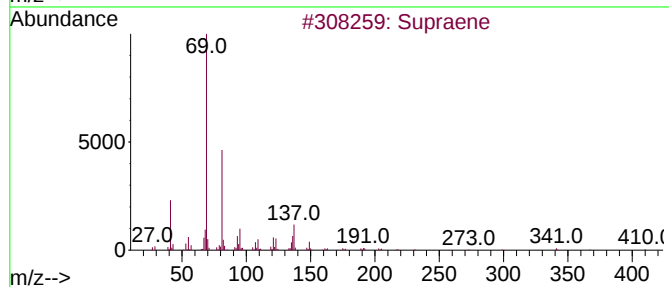
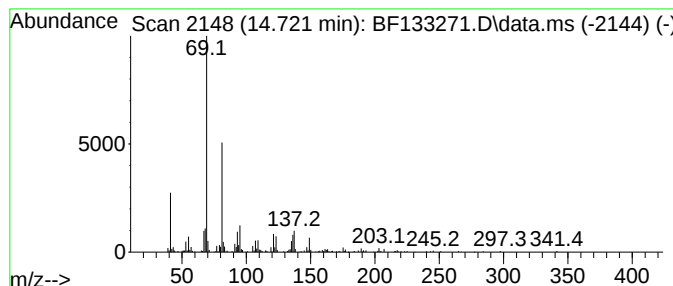
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.721	2.54 ng	162005	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133271.D
Acq On : 05 May 2023 19:17
Operator : CG\JU
Sample : 02618-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.910	7.5	ng	422911	1	6.722	1126440	20.0
Benzophenone	10.475	12.2	ng	1012590	3	9.757	1657920	20.0
Methanone, (1-h...	10.781	2.4	ng	209502	4	11.239	1724890	20.0
Dimethazone	11.004	5.1	ng	441801	4	11.239	1724890	20.0
n-Hexadecanoic ...	11.780	5.8	ng	496882	4	11.239	1724890	20.0
Dichloroacetic ...	13.733	4.1	ng	309323	5	13.874	1518140	20.0
Triphenylphosph...	13.969	12.9	ng	980770	5	13.874	1518140	20.0
Supraene	14.721	2.5	ng	162005	6	15.292	1276220	20.0