

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021225\
 Data File : BF141596.D
 Acq On : 12 Feb 2025 17:54
 Operator : RC/JU
 Sample : Q1348-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-1-WC

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-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.404	558	563	583	rBV	916986	1273609	41.70%	7.992%
2	6.422	729	736	762	rBV	546909	899955	29.47%	5.647%
3	6.787	793	798	805	rBV	386992	497444	16.29%	3.122%
4	6.851	805	809	821	rBV	34819	63596	2.08%	0.399%
5	7.351	885	894	904	rBV	1238990	1703317	55.77%	10.689%
6	7.451	904	911	922	rVB4	10695	38527	1.26%	0.242%
7	7.810	964	972	987	rBV3	21153	56012	1.83%	0.351%
8	7.992	996	1003	1011	rBV3	13480	39790	1.30%	0.250%
9	8.069	1011	1016	1031	rVB	488333	669876	21.93%	4.204%
10	8.422	1070	1076	1087	rBV	46244	100379	3.29%	0.630%
11	9.145	1193	1199	1210	rBV	2316013	3054050	100.00%	19.165%
12	9.251	1213	1217	1225	rVB2	43225	75566	2.47%	0.474%
13	9.822	1308	1314	1323	rBV	568477	736314	24.11%	4.621%
14	10.033	1345	1350	1361	rBV	86561	171339	5.61%	1.075%
15	10.228	1378	1383	1390	rVB2	23283	44068	1.44%	0.277%
16	10.533	1430	1435	1442	rBV	189025	240206	7.87%	1.507%
17	10.610	1442	1448	1463	rBV	1408594	1890998	61.92%	11.866%
18	10.986	1506	1512	1518	rBV4	13486	31416	1.03%	0.197%
19	11.304	1561	1566	1574	rBV	558113	728164	23.84%	4.569%
20	11.692	1626	1632	1636	rBV	79575	97807	3.20%	0.614%
21	11.845	1652	1658	1660	rBV3	30227	52862	1.73%	0.332%
22	12.892	1830	1836	1841	rBV	2022965	2609903	85.46%	16.378%
23	13.945	2010	2015	2026	rBV	314743	446551	14.62%	2.802%
24	15.410	2258	2264	2278	rBV	247380	413901	13.55%	2.597%

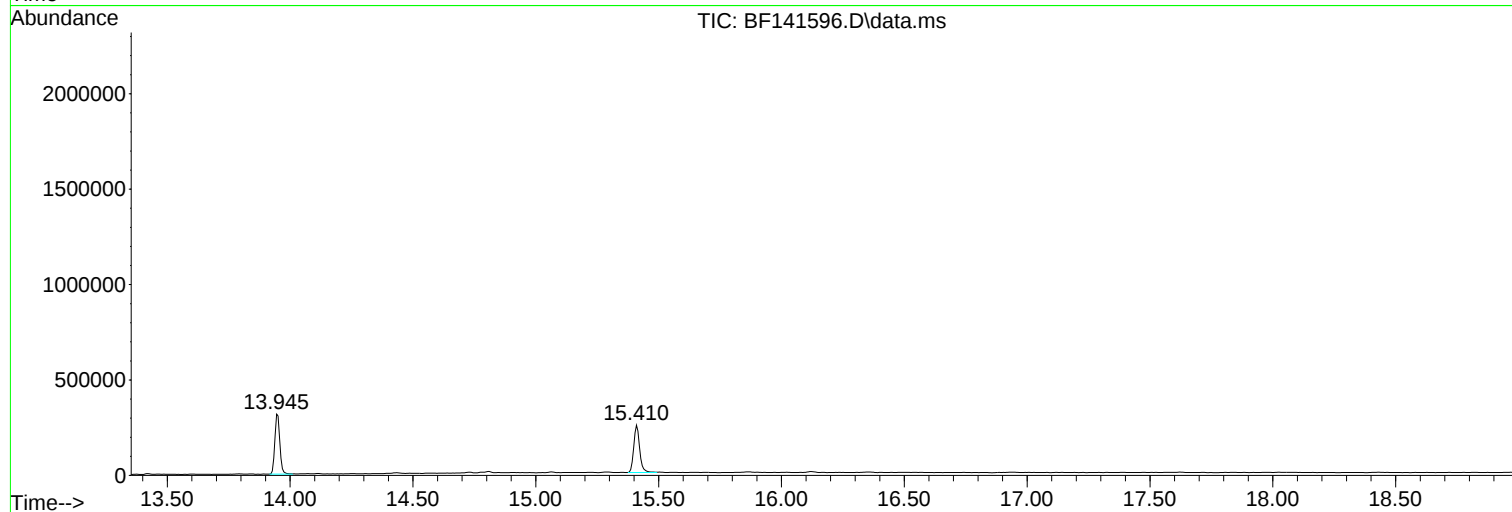
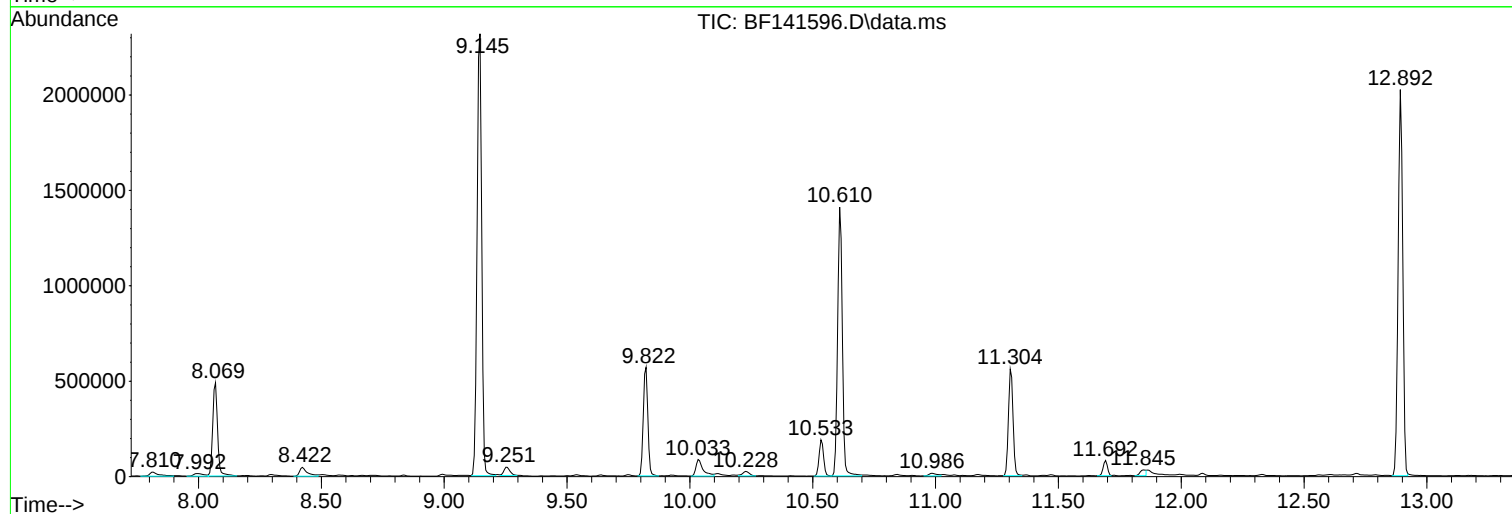
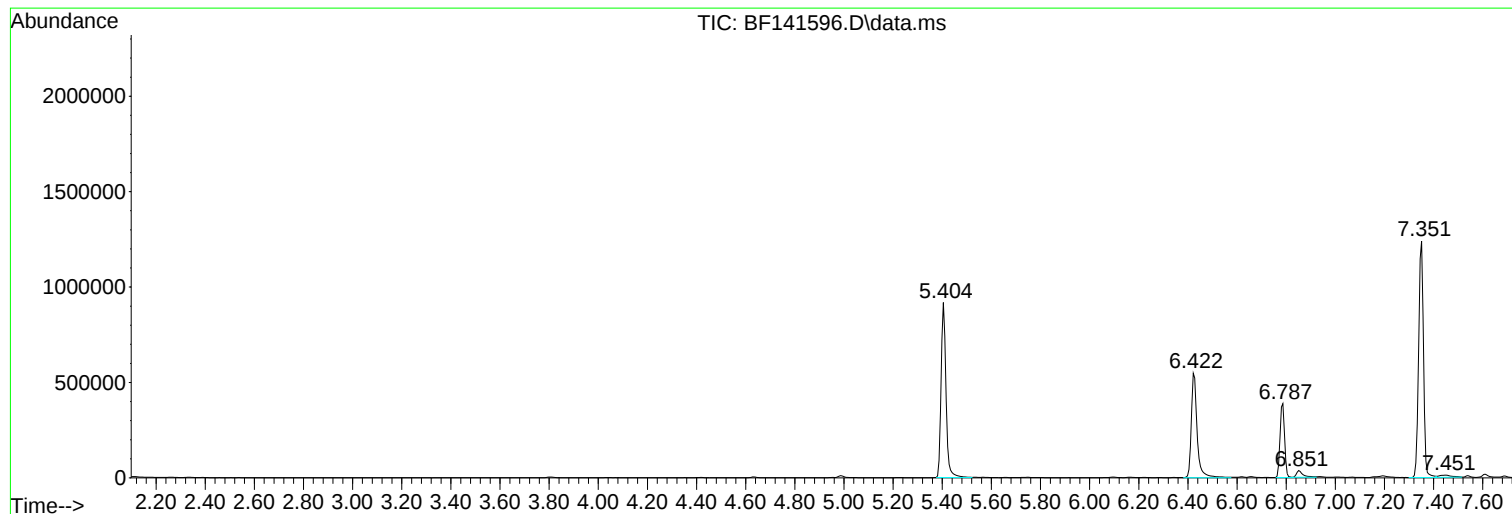
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TWP-1-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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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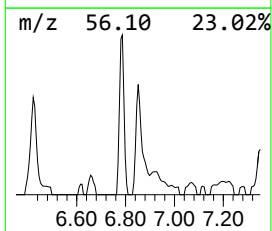
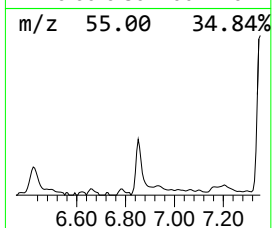
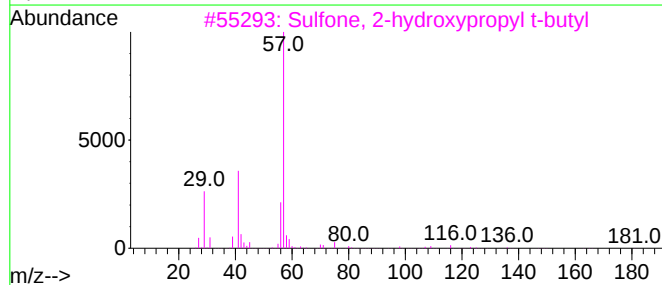
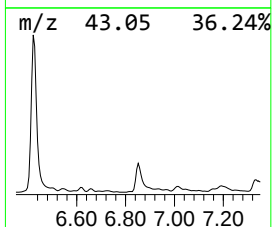
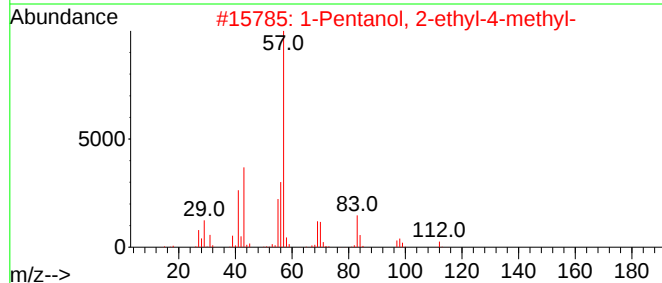
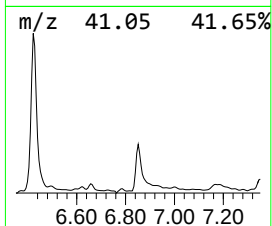
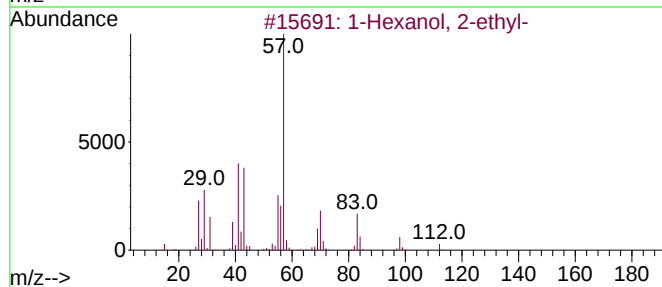
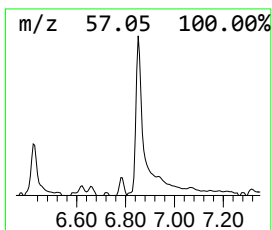
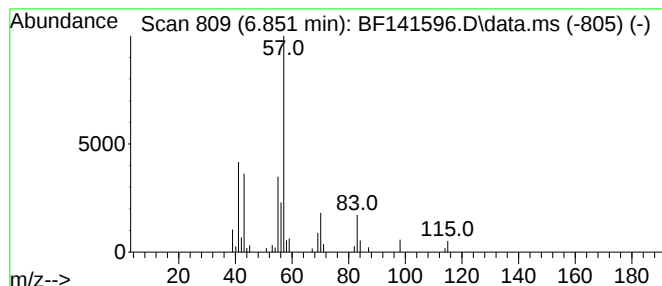
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.851	2.56 ng	63596	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
3			Sulfone, 2-hydroxypropyl t-butyl	180	C7H16O3S	154619-05-3	43
4			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	40



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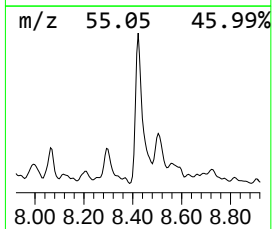
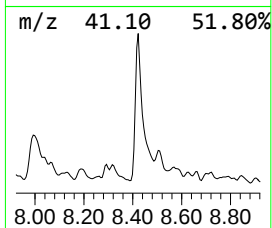
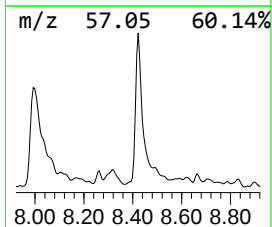
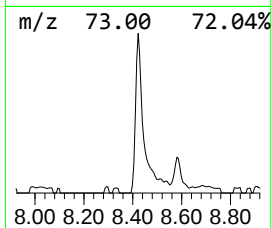
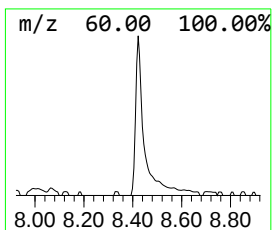
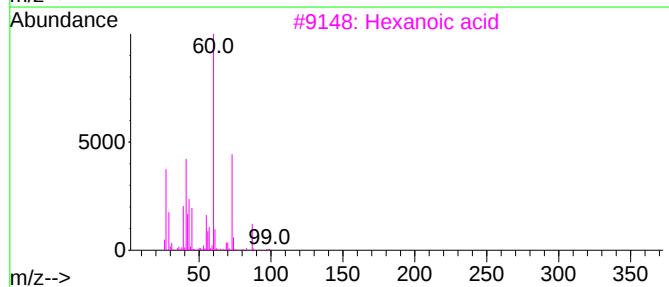
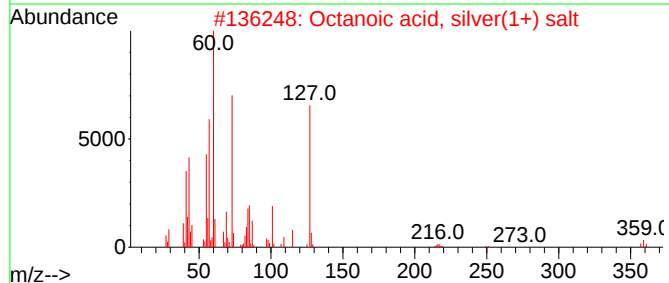
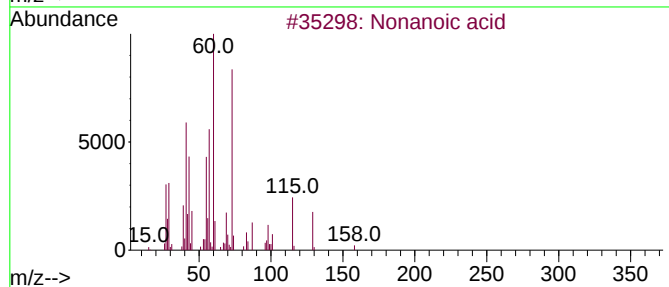
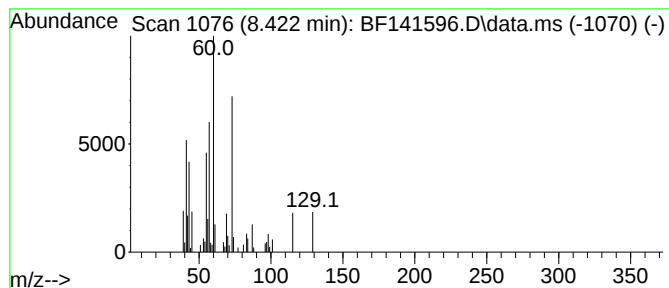
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Peak Number 2 Nonanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.422	3.00 ng	100379	Naphthalene-d8	8.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	90
2			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	59
3			Hexanoic acid	116	C6H12O2	000142-62-1	53
4			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	50
5			Butanoic acid	88	C4H8O2	000107-92-6	50



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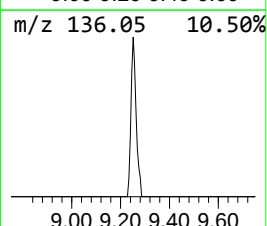
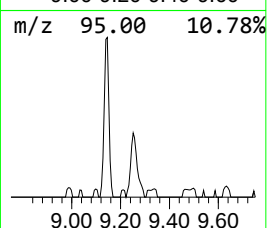
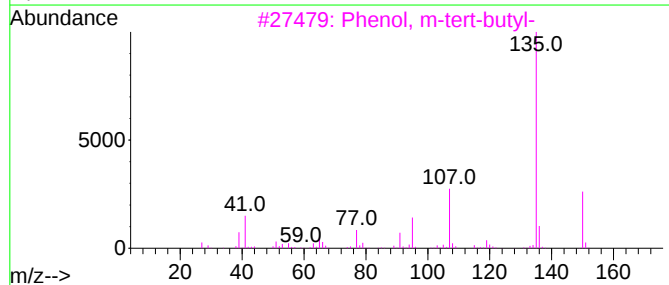
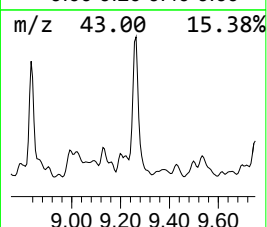
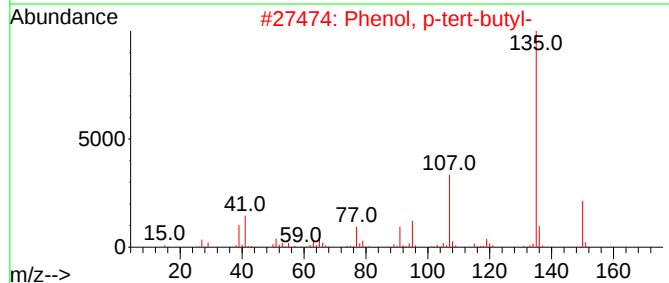
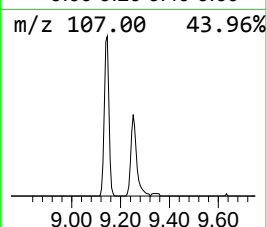
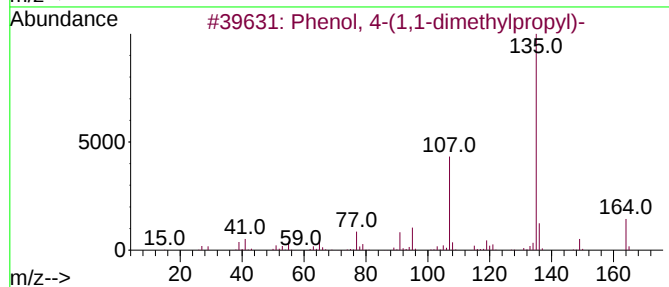
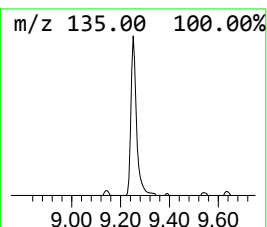
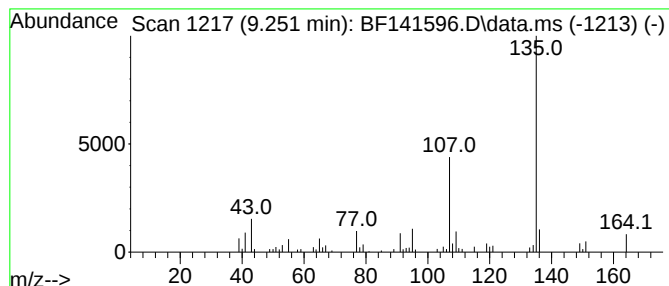
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Phenol, 4-(1,1-dimethylprop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.251	2.05 ng	75566	Acenaphthene-d10	9.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	80
3			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	68
4			Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64
5			Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	59



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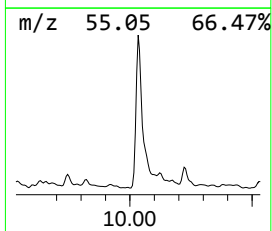
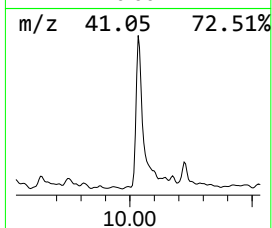
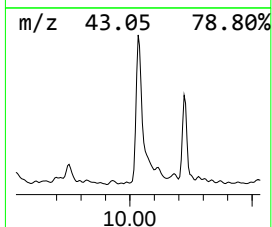
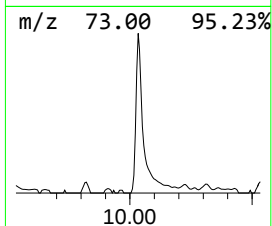
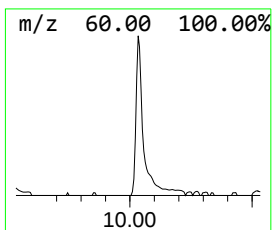
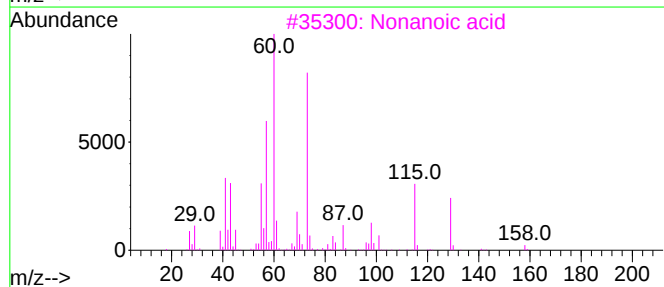
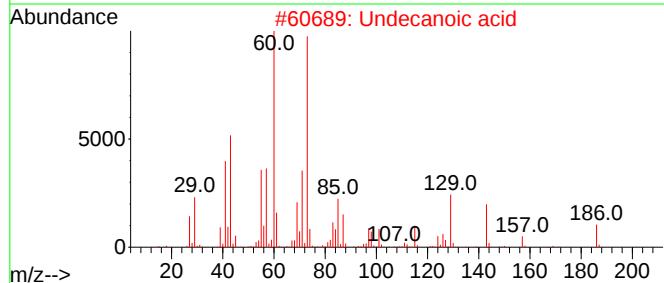
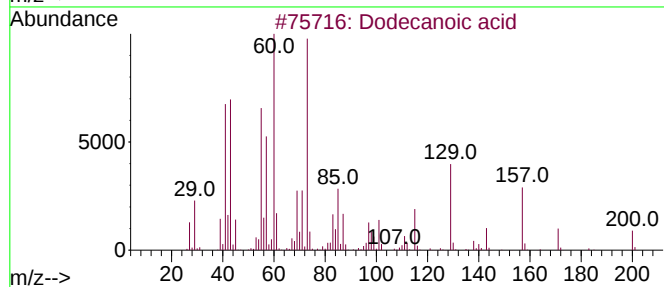
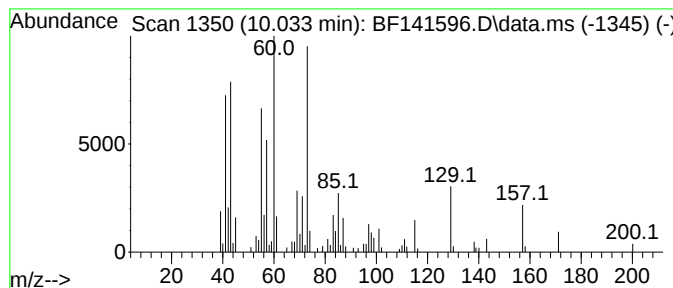
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.033	4.65 ng	171339	Acenaphthene-d10	9.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	97
2			Undecanoic acid	186	C11H22O2	000112-37-8	72
3			Nonanoic acid	158	C9H18O2	000112-05-0	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	47
5			.alpha.,.beta.-D-Glucopyranoside...	264	C12H24O6	1000158-67-6	43



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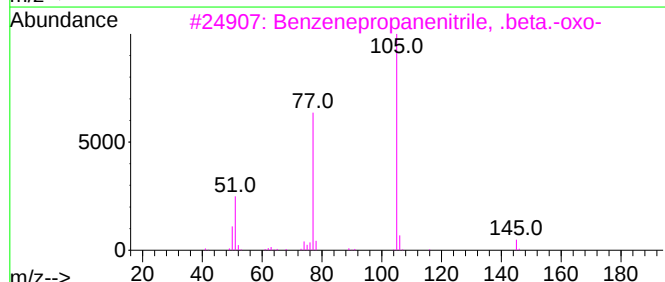
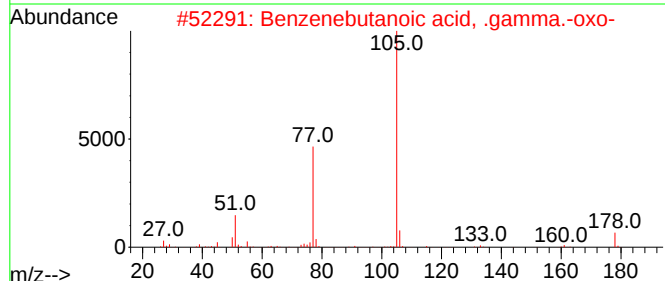
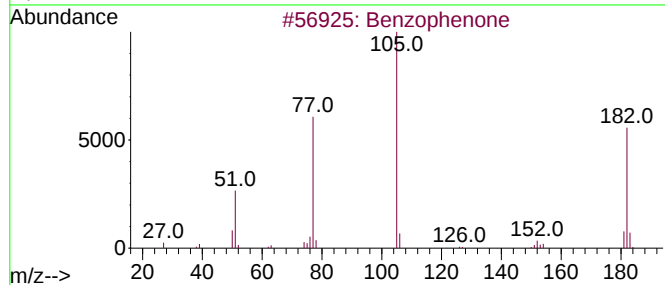
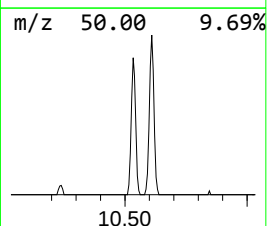
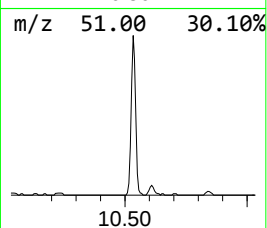
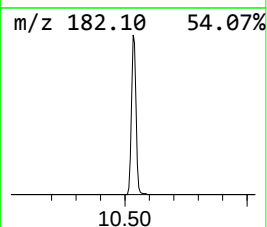
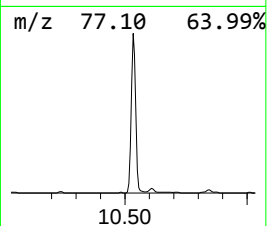
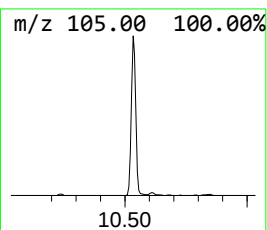
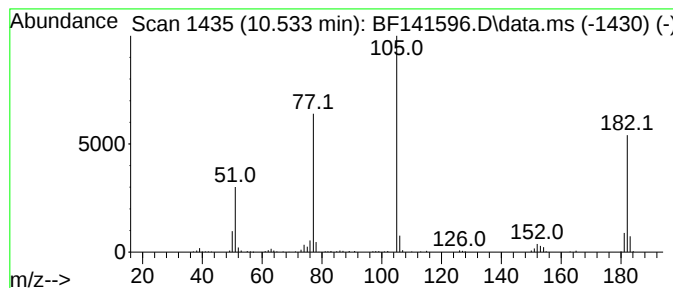
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.533	6.52 ng	240206	Acenaphthene-d10	9.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
3			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50



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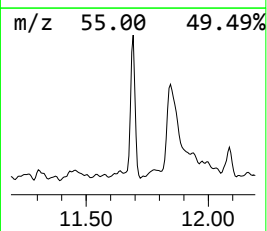
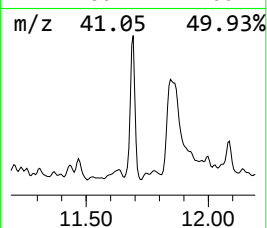
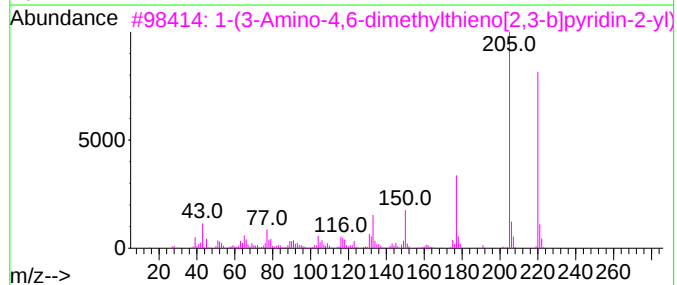
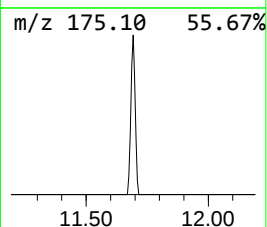
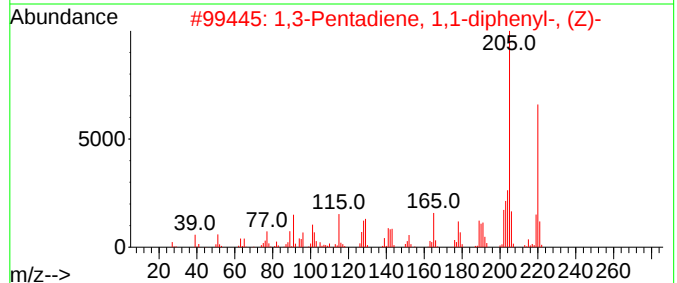
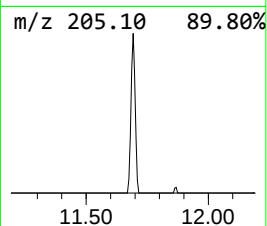
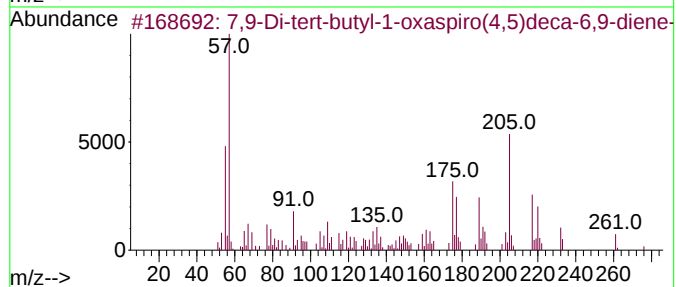
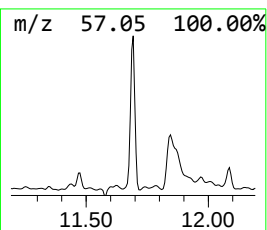
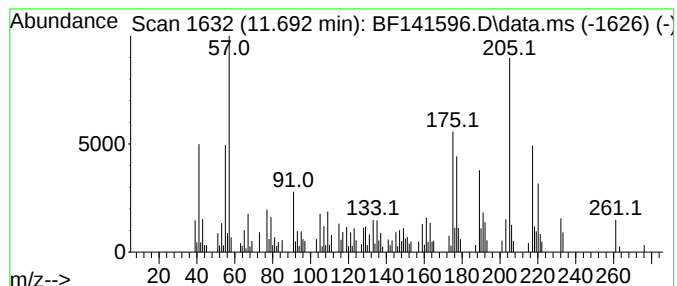
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.692	2.69 ng	97807	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	49		
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	49		
4	3H-Cyclopenta[1,3]cyclopropa[1,2...	220	C14H20O2	066708-18-7	46		
5	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	44		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021225\
Data File : BF141596.D
Acq On : 12 Feb 2025 17:54
Operator : RC/JU
Sample : Q1348-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-1-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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
1-Hexanol, 2-et...	6.851	2.6	ng	63596	1	6.787	497444	20.0
Nonanoic acid	8.422	3.0	ng	100379	2	8.069	669876	20.0
Phenol, 4-(1,1-...	9.251	2.0	ng	75566	3	9.822	736314	20.0
Dodecanoic acid	10.033	4.7	ng	171339	3	9.822	736314	20.0
Benzophenone	10.533	6.5	ng	240206	3	9.822	736314	20.0
7,9-Di-tert-but...	11.692	2.7	ng	97807	4	11.304	728164	20.0