

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113023\
 Data File : BF136326.D
 Acq On : 30 Nov 2023 21:49
 Operator : CG\JU
 Sample : 05434-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	496	502	507	rBV	20534	26519	1.33%	0.190%
2	5.440	566	570	573	rBV	1803170	1505350	75.74%	10.763%
3	6.440	735	740	743	rBV	1532157	1315735	66.20%	9.407%
4	6.640	770	774	779	rBV	21922	27959	1.41%	0.200%
5	6.804	799	802	806	rBV	683987	558527	28.10%	3.993%
6	7.363	893	897	900	rBV	1060809	840142	42.27%	6.007%
7	8.081	1015	1019	1023	rBV	733922	621383	31.26%	4.443%
8	9.157	1199	1202	1206	rBV	1762266	1548206	77.90%	11.069%
9	9.839	1314	1318	1322	rBV	826382	639598	32.18%	4.573%
10	10.628	1449	1452	1464	rVB	1056015	964949	48.55%	6.899%
11	10.769	1471	1476	1479	rBV2	31057	34076	1.71%	0.244%
12	10.816	1481	1484	1487	rBV	85300	80745	4.06%	0.577%
13	10.851	1487	1490	1494	rVV2	87085	115226	5.80%	0.824%
14	10.886	1494	1496	1498	rVV	89511	80590	4.05%	0.576%
15	10.910	1498	1500	1503	rVV	50801	47629	2.40%	0.341%
16	10.939	1503	1505	1508	rVV2	27960	42822	2.15%	0.306%
17	10.998	1512	1515	1519	rVV3	68263	86202	4.34%	0.616%
18	11.039	1519	1522	1524	rVV	83882	93278	4.69%	0.667%
19	11.075	1526	1528	1534	rVB	55612	64627	3.25%	0.462%
20	11.333	1568	1572	1574	rBV	881801	723831	36.42%	5.175%
21	11.357	1574	1576	1579	rVV	147955	118005	5.94%	0.844%
22	11.404	1579	1584	1587	rVB	48438	52878	2.66%	0.378%
23	11.733	1636	1640	1644	rVB7	16595	23886	1.20%	0.171%
24	11.798	1645	1651	1655	rBV4	19083	36563	1.84%	0.261%
25	11.833	1655	1657	1660	rBV	21443	22945	1.15%	0.164%
26	11.869	1660	1663	1667	rBV	242886	215829	10.86%	1.543%
27	11.951	1673	1677	1679	rBV	33930	40759	2.05%	0.291%
28	12.551	1775	1779	1782	rBV	287559	265053	13.34%	1.895%
29	12.657	1794	1797	1802	rBV2	66132	81230	4.09%	0.581%
30	12.780	1812	1818	1821	rBV	238987	252572	12.71%	1.806%
31	12.816	1822	1824	1831	rVB2	52184	88301	4.44%	0.631%
32	12.927	1839	1843	1847	rBV	2150013	1987537	100.00%	14.210%
33	12.980	1850	1852	1854	rBV2	24027	24798	1.25%	0.177%
34	13.110	1872	1874	1877	rVB	48904	45397	2.28%	0.325%
35	13.986	2019	2023	2026	rBV	786263	777985	39.14%	5.562%
36	15.474	2272	2276	2284	rVB	355258	535290	26.93%	3.827%

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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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

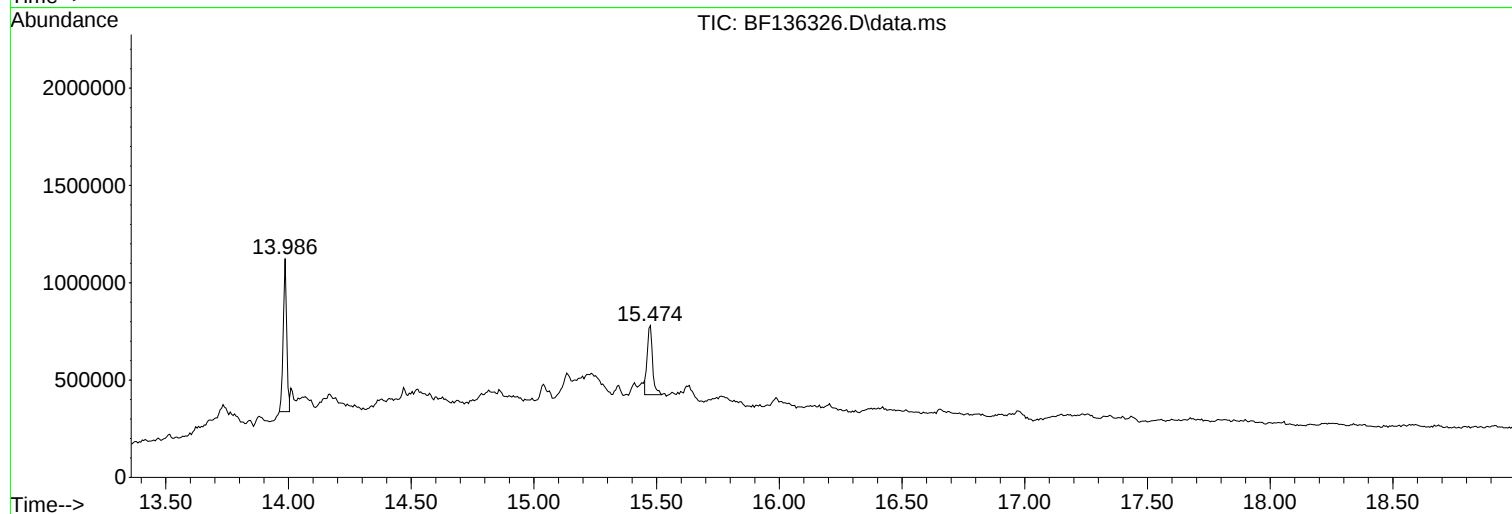
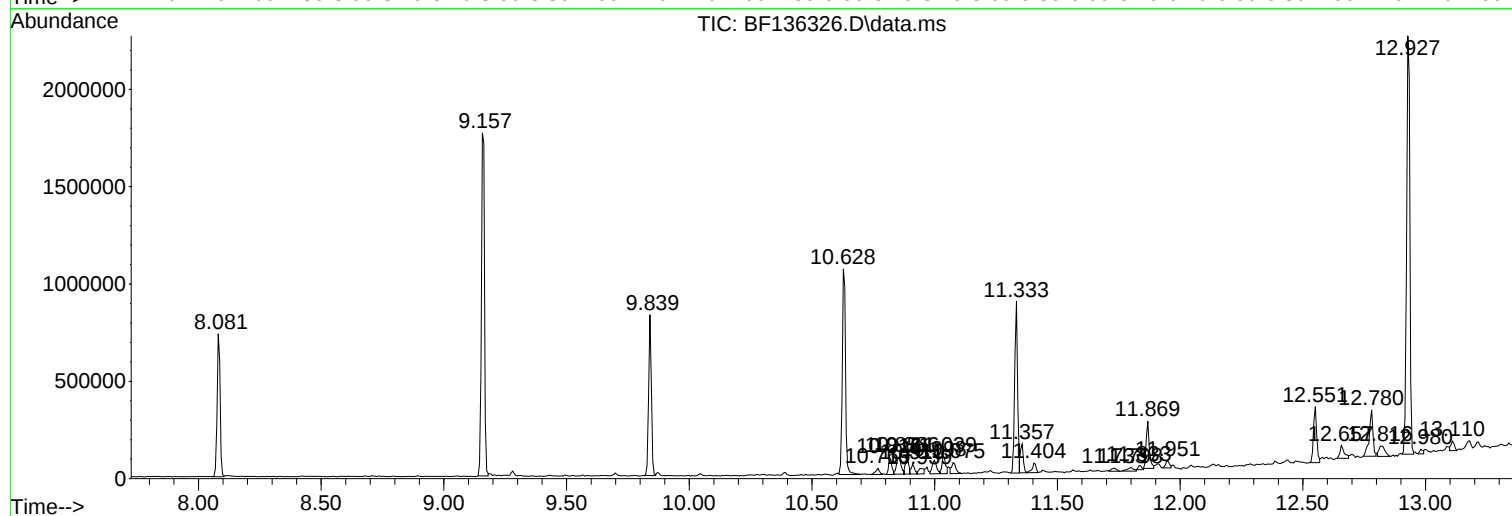
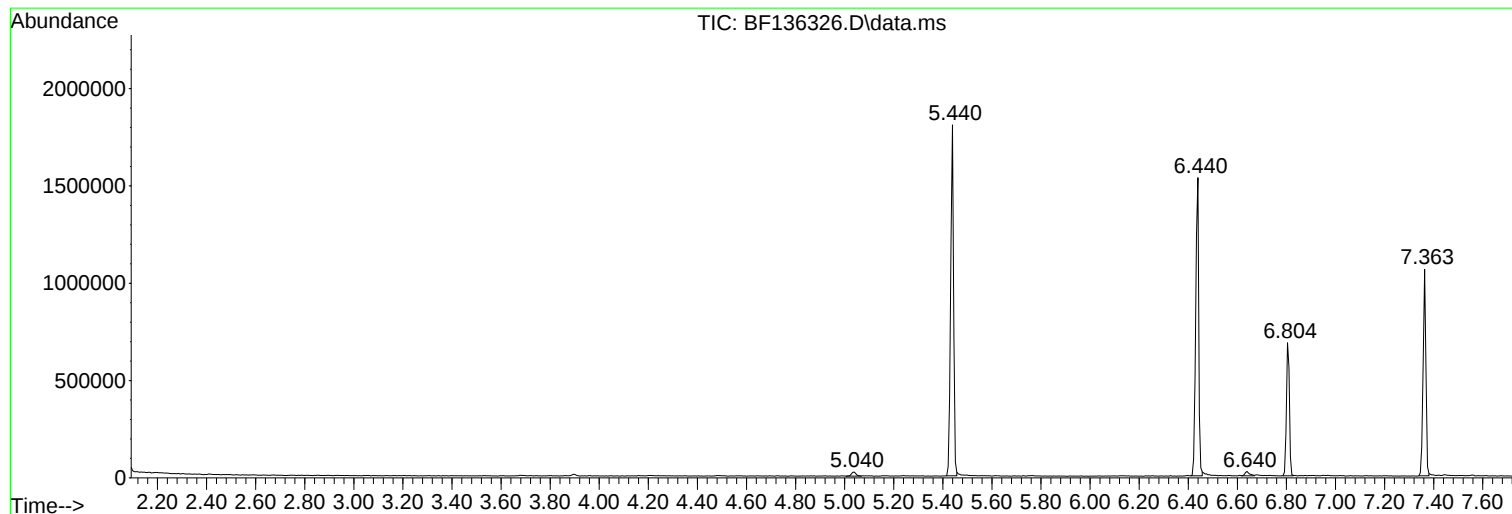
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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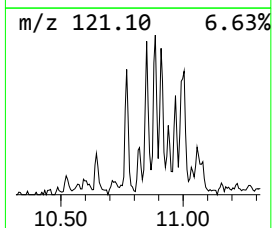
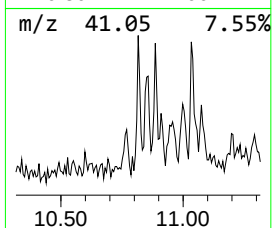
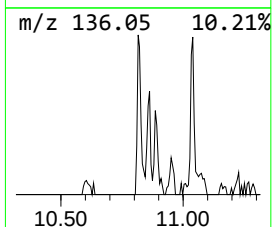
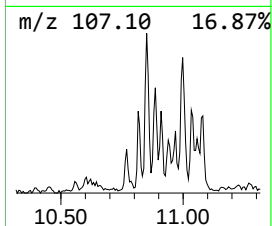
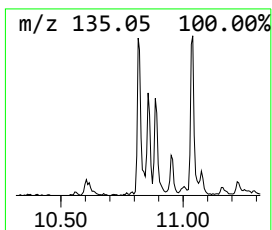
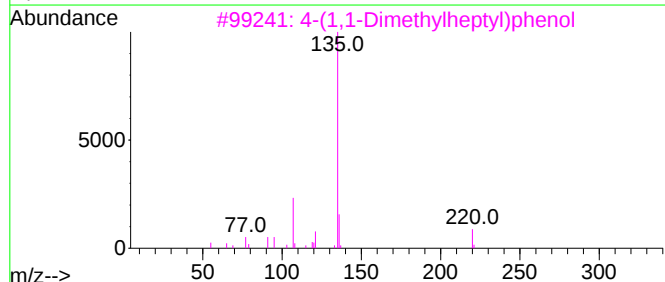
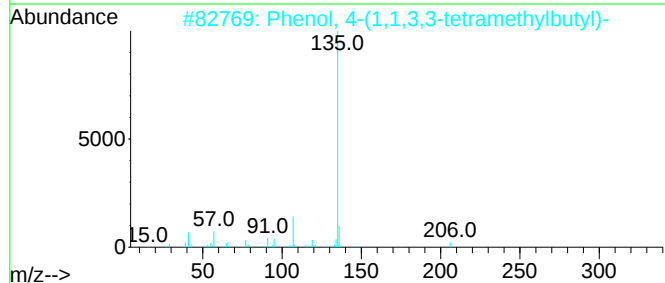
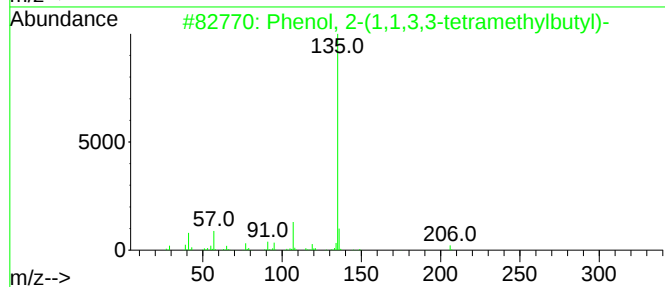
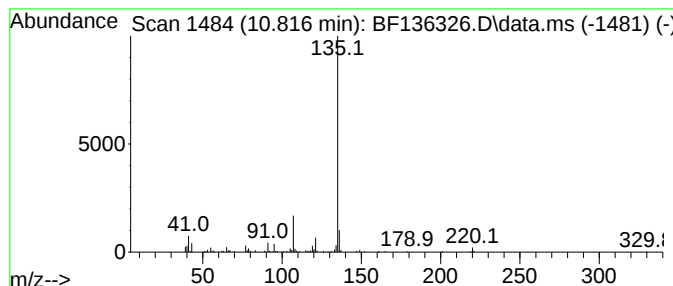
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Phenol, 2-(1,1,3,3-tetramet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.816	2.23 ng	80745	Phenanthrene-d10	11.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	86
2			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	86
3			4-(1,1-Dimethylheptyl)phenol	220	C15H24O	1000384-80-3	83
4			4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
5			Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	000459-22-3	72



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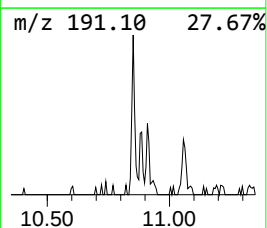
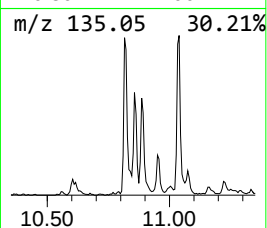
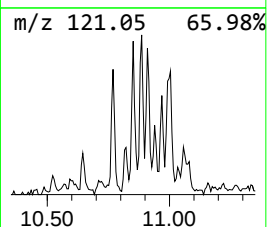
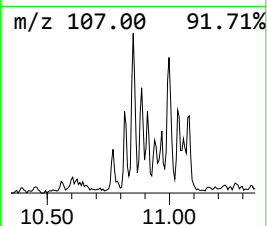
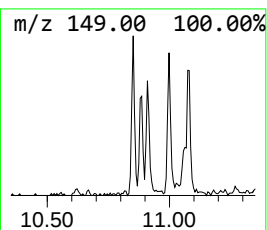
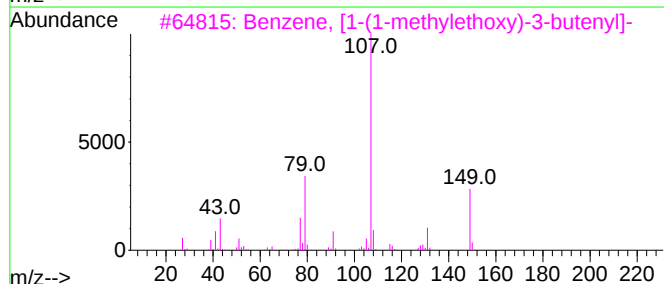
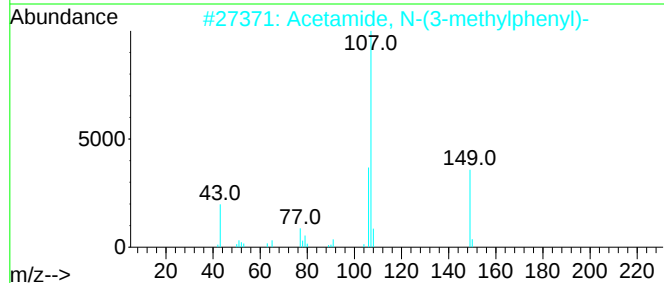
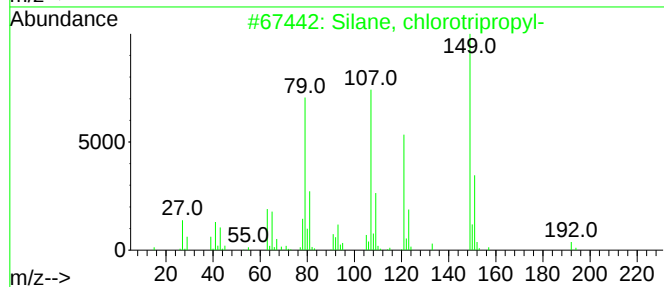
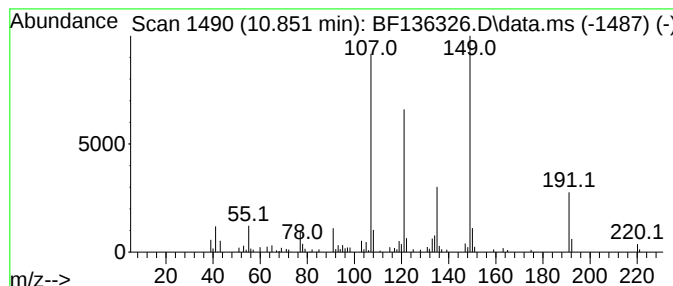
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Silane, chlorotripropyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	3.18 ng	115226	Phenanthrene-d10	11.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, chlorotripropyl-	192	C9H21ClSi	000995-25-5	64
2			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	58
3			Benzene, [1-(1-methylethoxy)-3-b...	190	C13H18O	098088-47-2	53
4			5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	38
5			Butanamide, N-(2-methylphenyl)-3...	191	C11H13NO2	000093-68-5	38



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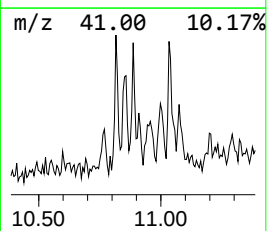
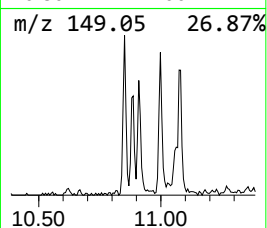
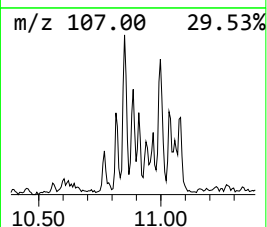
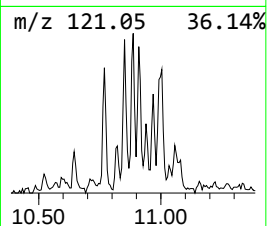
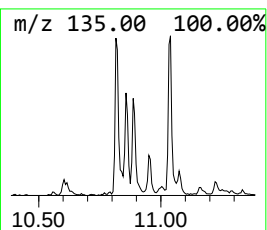
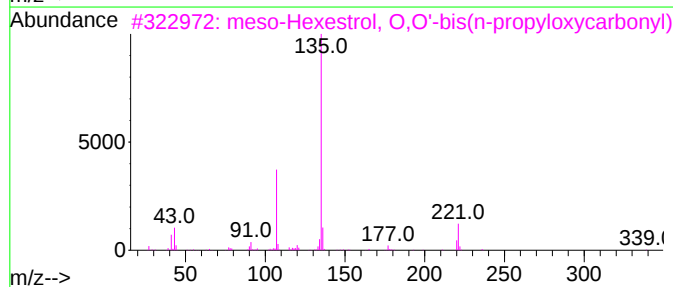
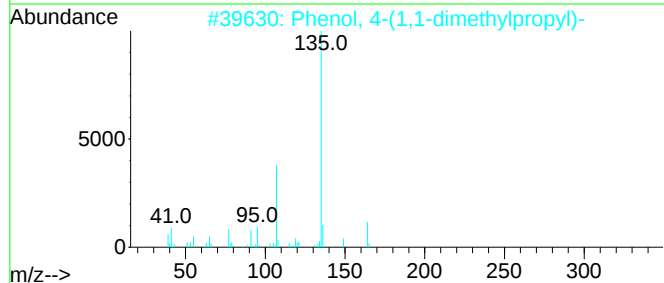
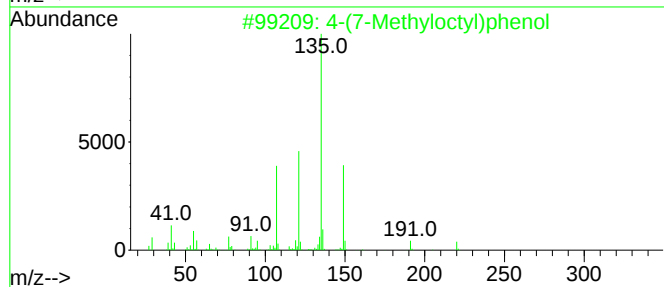
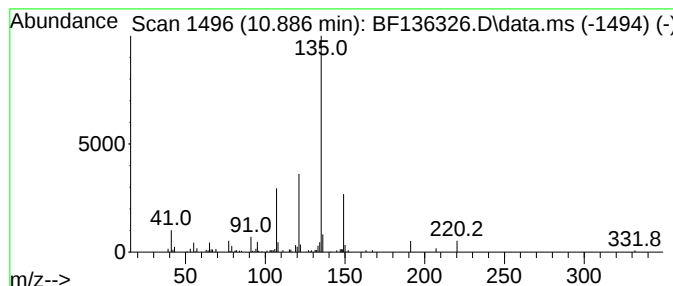
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4-(7-Methyloctyl)phenol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.886	2.23 ng	80590	Phenanthrene-d10	11.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	98
2			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	59
3			meso-Hexestrol, O,O'-bis(n-propy...	442	C26H34O6	1000487-65-0	59
4			meso-Hexestrol, O,O'-bis(ethoxyc...	414	C24H30O6	1000487-68-5	53
5			Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	53



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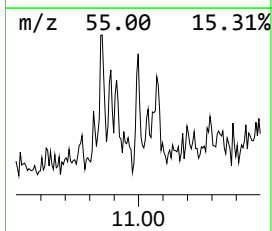
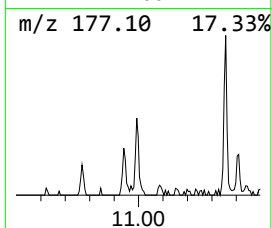
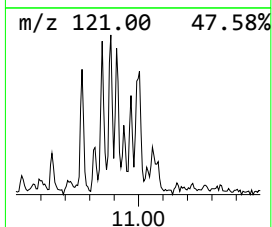
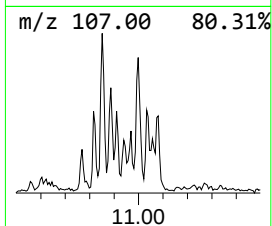
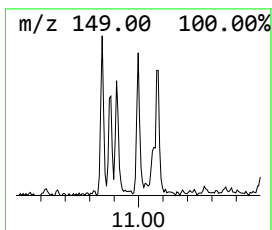
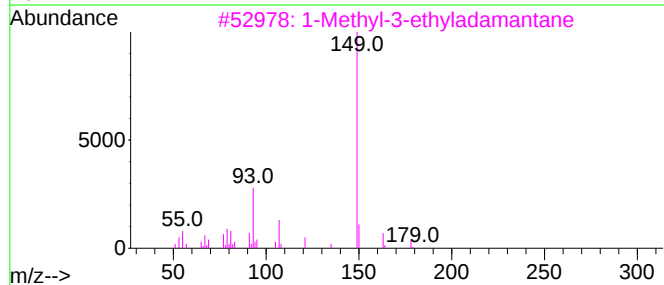
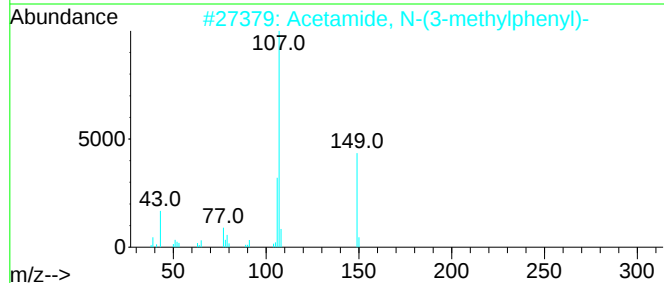
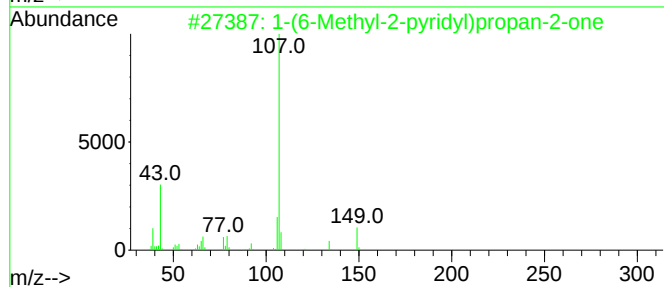
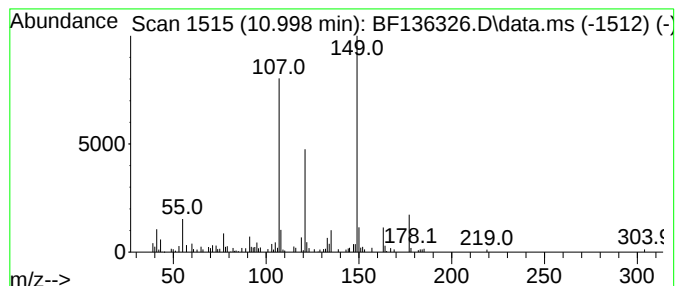
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-(6-Methyl-2-pyridyl)propa... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.998	2.38 ng	86202	Phenanthrene-d10	11.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	72
2			Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	49
3			1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	47
4			Isobutyramide, N-methyl-N-phenyl-	177	C11H15NO	1000339-96-1	38
5			Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	38



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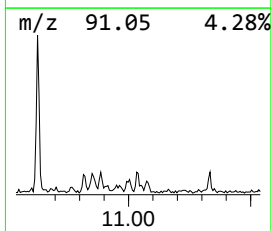
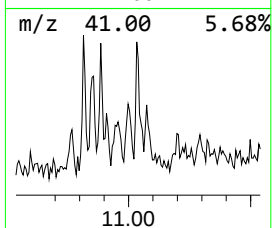
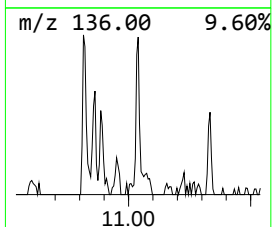
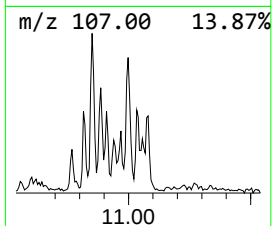
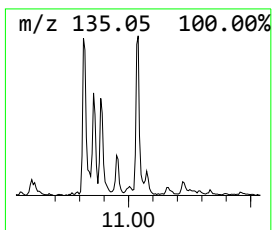
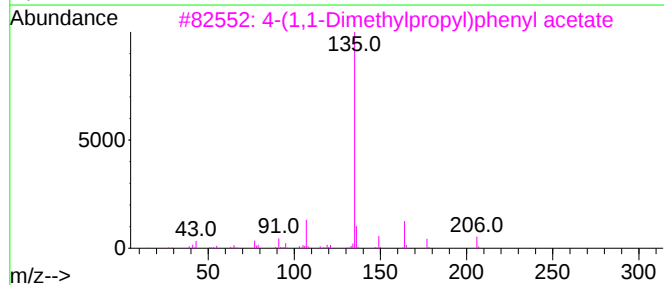
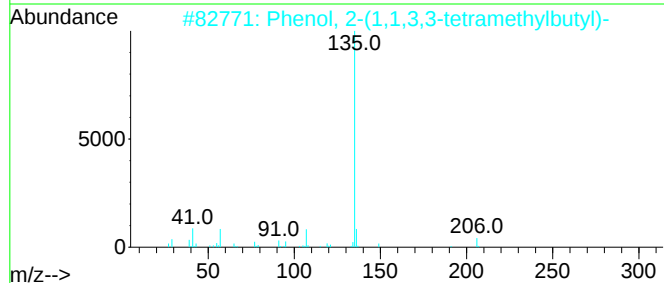
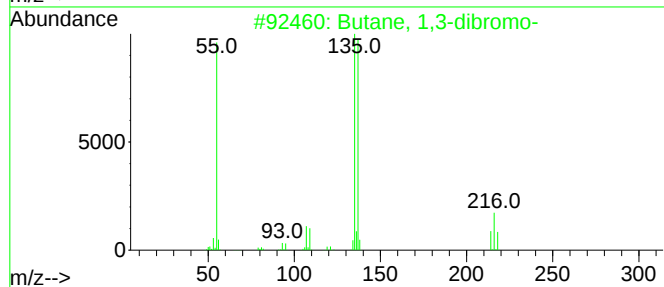
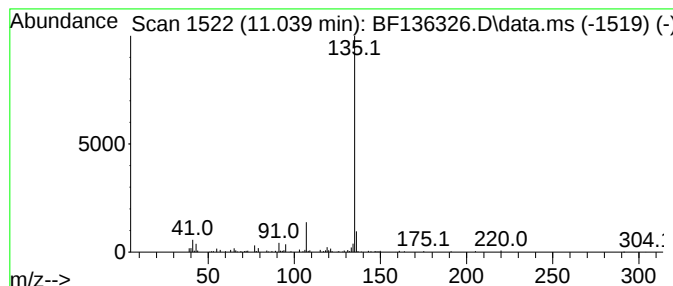
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Butane, 1,3-dibromo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.039	2.58 ng	93278	Phenanthrene-d10	11.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1,3-dibromo-	214	C4H8Br2	000107-80-2	83
2			Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	78
3			4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
4			4-tert-Butylphenol, 0-(n-propylo...	236	C14H20O3	1000487-25-4	78
5			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113023\
Data File : BF136326.D
Acq On : 30 Nov 2023 21:49
Operator : CG\JU
Sample : 05434-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

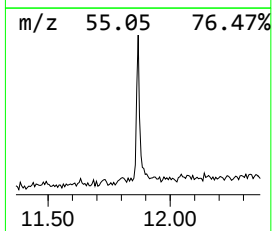
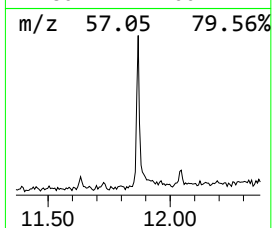
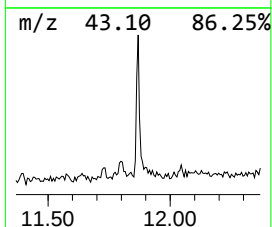
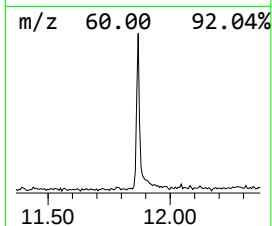
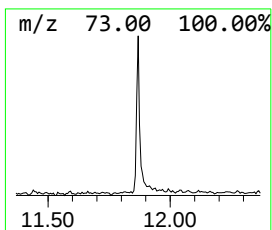
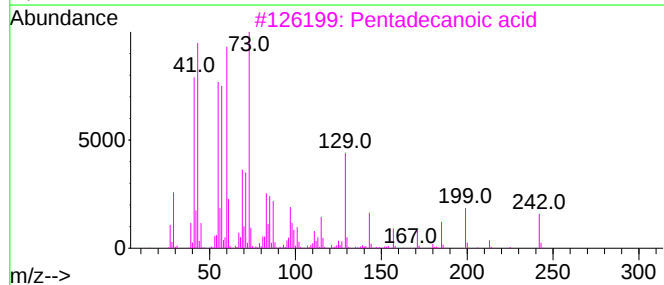
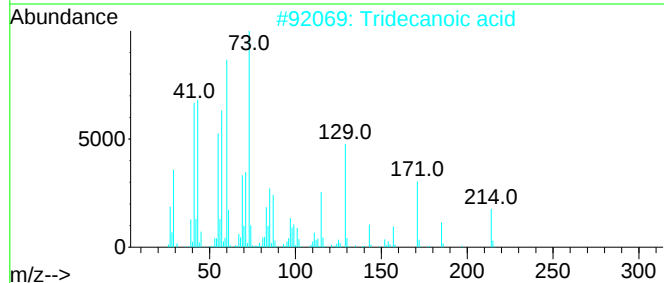
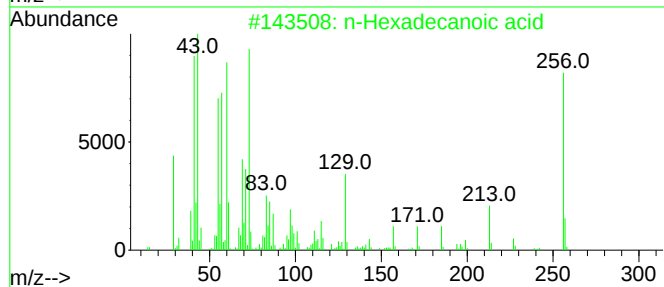
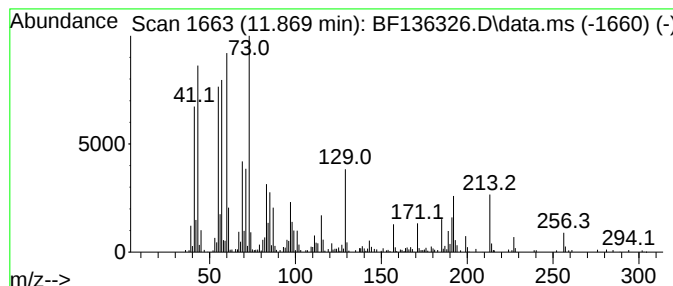
Instrument :
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ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.869	5.96 ng	215829	Phenanthrene-d10	11.333	
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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113023\
Data File : BF136326.D
Acq On : 30 Nov 2023 21:49
Operator : CG\JU
Sample : 05434-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

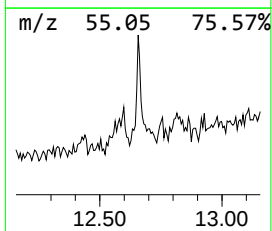
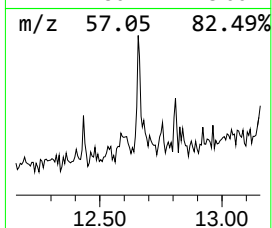
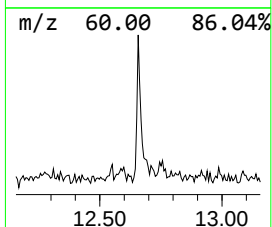
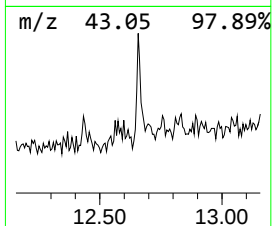
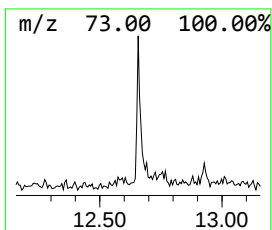
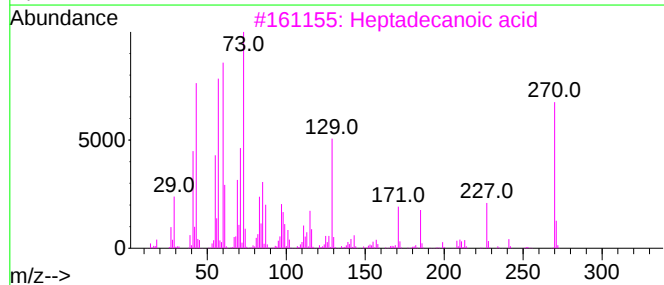
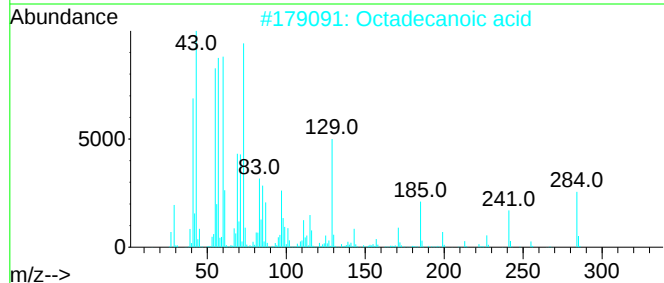
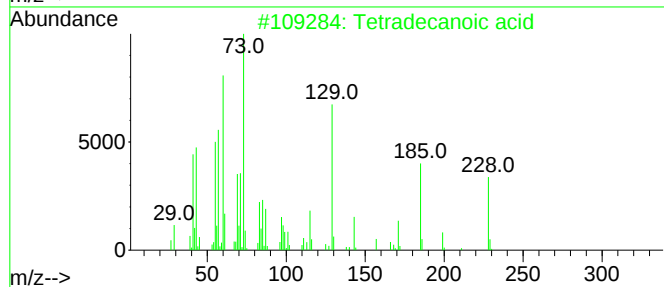
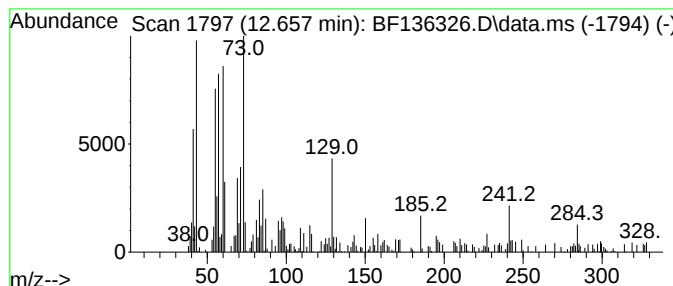
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.657	2.24 ng	81230	Phenanthrene-d10		11.333	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetradecanoic acid		228	C14H28O2	000544-63-8	97
2	Octadecanoic acid		284	C18H36O2	000057-11-4	95
3	Heptadecanoic acid		270	C17H34O2	000506-12-7	95
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
5	Tridecanoic acid		214	C13H26O2	000638-53-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113023\
Data File : BF136326.D
Acq On : 30 Nov 2023 21:49
Operator : CG\JU
Sample : 05434-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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
Phenol, 2-(1,1,...	10.816	2.2	ng	80745	4	11.333	723831	20.0
Silane, chlorot...	10.851	3.2	ng	115226	4	11.333	723831	20.0
4-(7-Methylocty...	10.886	2.2	ng	80590	4	11.333	723831	20.0
1-(6-Methyl-2-p...	10.998	2.4	ng	86202	4	11.333	723831	20.0
Butane, 1,3-dib...	11.039	2.6	ng	93278	4	11.333	723831	20.0
n-Hexadecanoic ...	11.869	6.0	ng	215829	4	11.333	723831	20.0
Tetradecanoic acid	12.657	2.2	ng	81230	4	11.333	723831	20.0