

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
 Data File : BF138561.D
 Acq On : 12 Jul 2024 22:41
 Operator : CG\JU
 Sample : P3183-07 10X
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-229

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-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138561.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.110	3	4	10	rVB	270696	235051	38.40%	4.811%
2	3.928	309	313	320	rVB2	8105	12686	2.07%	0.260%
3	5.069	504	507	512	rVB	26807	26148	4.27%	0.535%
4	5.487	575	578	588	rBV	167813	156607	25.58%	3.205%
5	6.498	747	750	758	rBV	178404	152715	24.95%	3.126%
6	6.869	809	813	816	rBV	600377	493300	80.59%	10.096%
7	7.422	904	907	911	rBV	103417	88782	14.50%	1.817%
8	8.145	1027	1030	1034	rVB	625136	528675	86.37%	10.820%
9	8.733	1127	1130	1134	rBV	14978	11088	1.81%	0.227%
10	9.222	1209	1213	1216	rBV	185879	152319	24.88%	3.117%
11	9.298	1221	1226	1229	rBV	27488	23785	3.89%	0.487%
12	9.616	1276	1280	1283	rBV5	12683	15131	2.47%	0.310%
13	9.828	1311	1316	1320	rVB	29965	26103	4.26%	0.534%
14	9.898	1325	1328	1332	rVV	619596	547278	89.40%	11.201%
15	9.998	1340	1345	1350	rVB8	7495	13480	2.20%	0.276%
16	10.145	1367	1370	1374	rBV6	9204	12297	2.01%	0.252%
17	10.327	1398	1401	1404	rVB	26892	20766	3.39%	0.425%
18	10.545	1434	1438	1440	rBV	14057	16162	2.64%	0.331%
19	10.686	1460	1462	1467	rBV	87692	70454	11.51%	1.442%
20	10.810	1478	1483	1490	rVB2	29604	47824	7.81%	0.979%
21	11.122	1531	1536	1538	rBV7	6659	8952	1.46%	0.183%
22	11.245	1554	1557	1560	rBV	24576	20262	3.31%	0.415%
23	11.274	1560	1562	1568	rVB2	19778	22764	3.72%	0.466%
24	11.386	1577	1581	1584	rBV	780013	612139	100.00%	12.528%
25	11.410	1584	1585	1589	rVB	23648	15968	2.61%	0.327%
26	11.622	1618	1621	1625	rBV6	9040	12328	2.01%	0.252%
27	11.674	1627	1630	1632	rVB	21382	18515	3.02%	0.379%
28	11.904	1663	1669	1675	rBV3	22840	45189	7.38%	0.925%
29	12.022	1682	1689	1693	rBV3	40065	71248	11.64%	1.458%
30	12.080	1696	1699	1701	rVV	25033	21399	3.50%	0.438%
31	12.186	1713	1717	1720	rBV	144891	124217	20.29%	2.542%
32	12.469	1762	1765	1768	rBV2	30937	27015	4.41%	0.553%
33	12.598	1784	1787	1789	rBV2	38762	36508	5.96%	0.747%
34	12.827	1824	1826	1830	rVB2	44733	51353	8.39%	1.051%
35	12.969	1847	1850	1853	rBV	225144	202145	33.02%	4.137%
36	14.021	2026	2029	2033	rBV	531915	480295	78.46%	9.830%

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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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.492	2276	2279	2289	rVB	324662	465119	75.98%	9.519%
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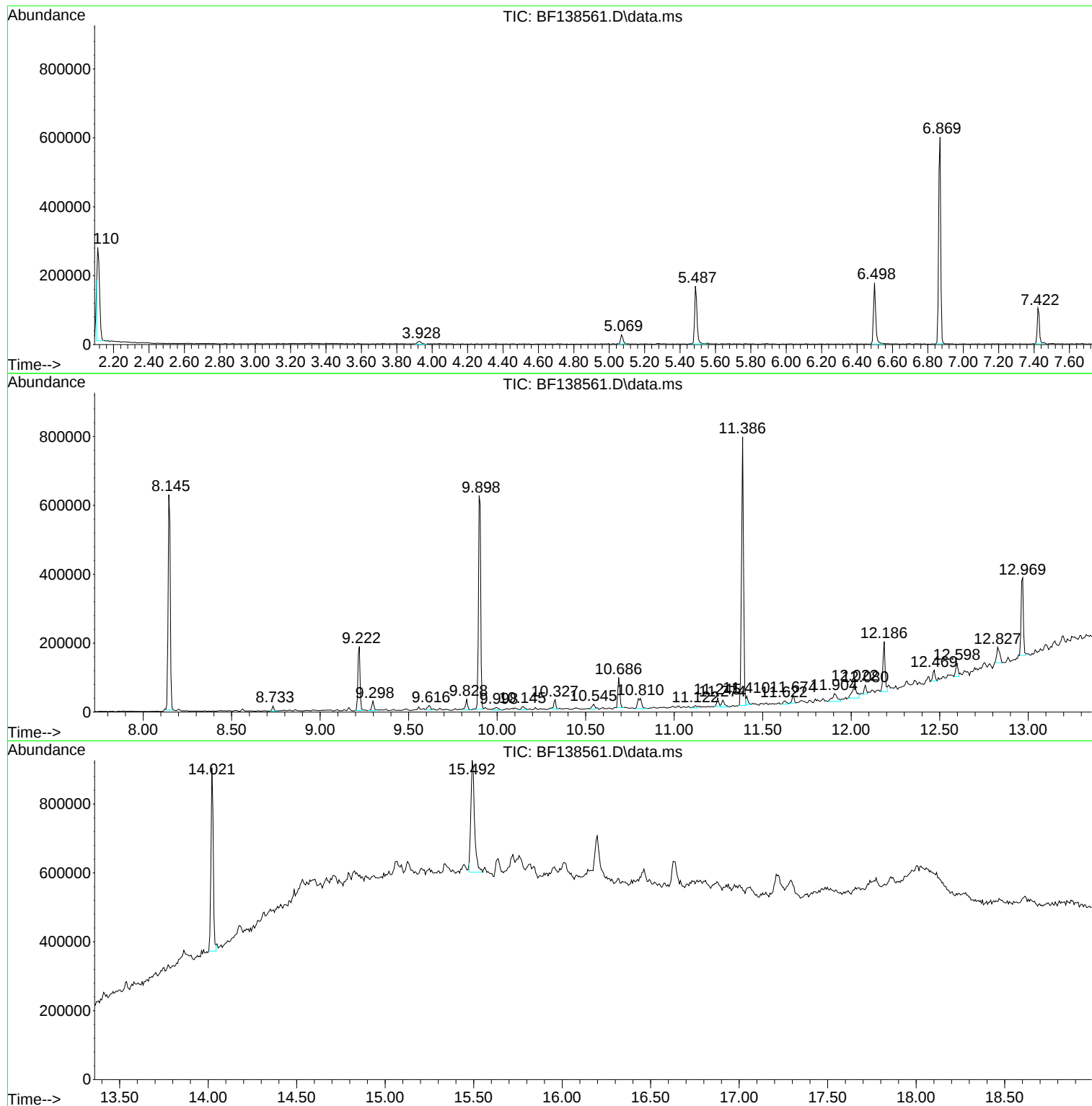
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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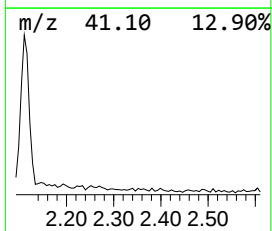
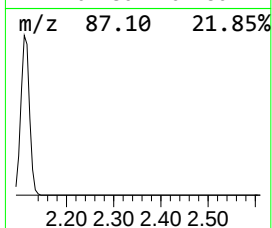
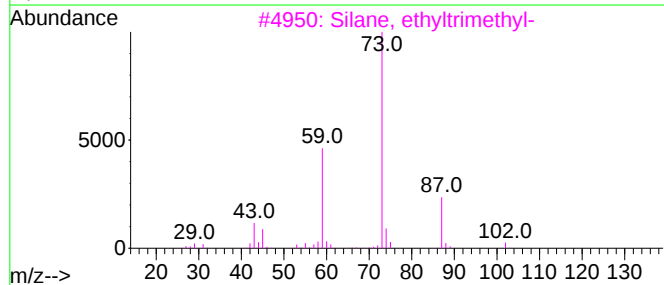
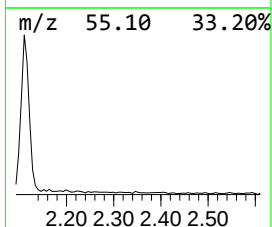
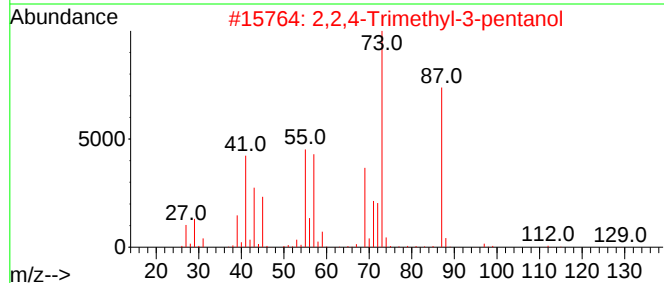
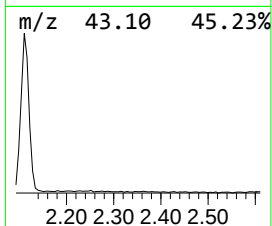
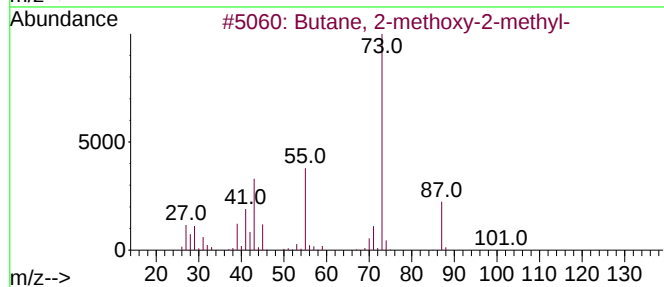
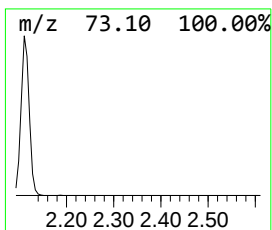
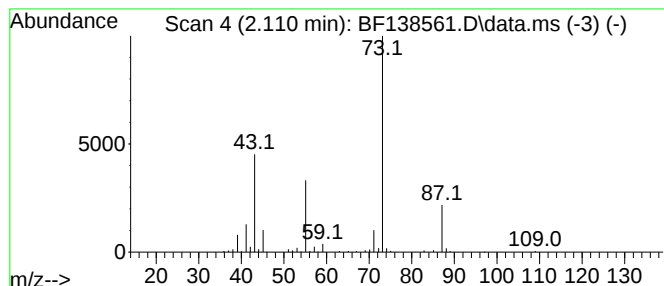
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.110	9.53 ng	235051	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Scyllo-Inositol, 1-C-methyl-	194	C7H14O6	000564-92-1	9



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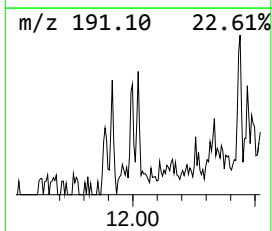
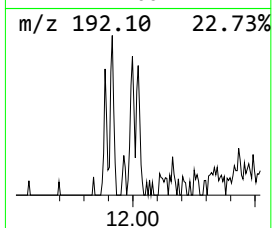
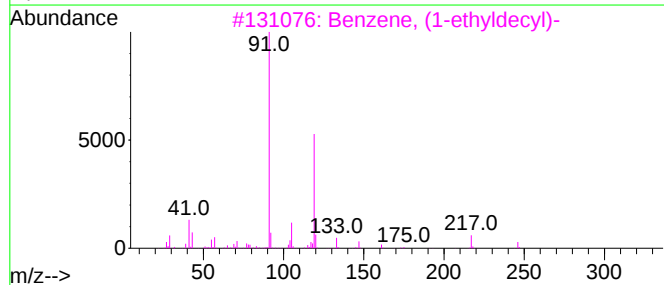
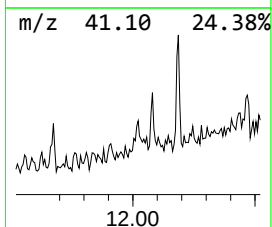
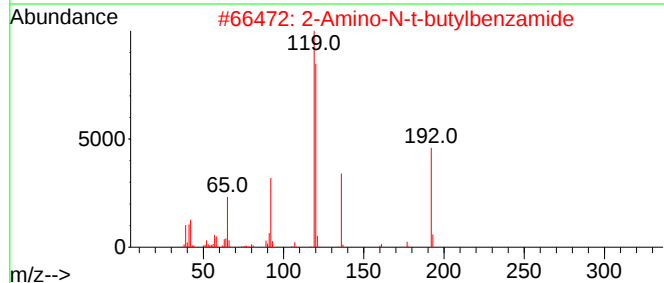
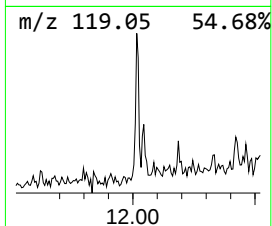
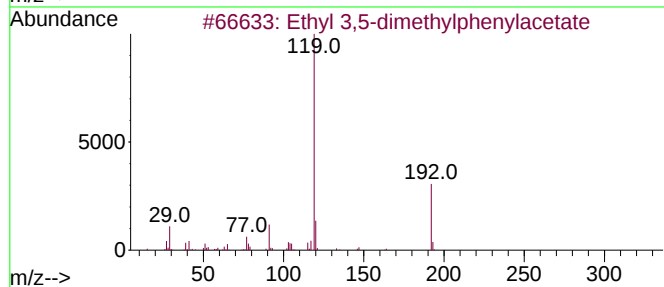
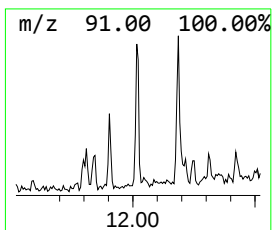
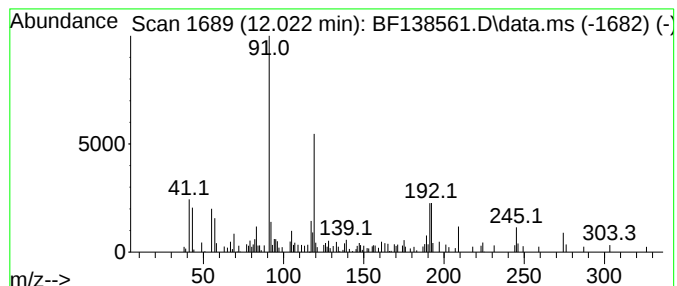
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown12.022 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	2.33 ng	71248	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl 3,5-dimethylphenylacetate	192	C12H16O2	105337-18-6	35
2			2-Amino-N-t-butylbenzamide	192	C11H16N2O	001203-89-0	35
3			Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	22
4			Benzamide, 4-methyl-N-(2-butyl)-...	303	C20H33NO	1000464-12-2	22
5			1,3-Dioxolan-2-one, 4-methyl-5-m...	246	C15H18O3	1000319-92-8	22



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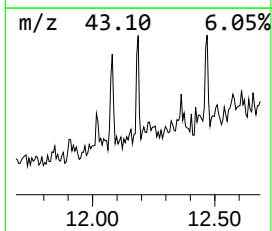
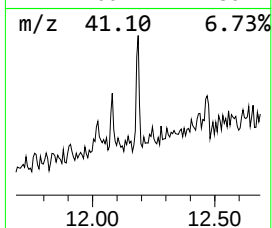
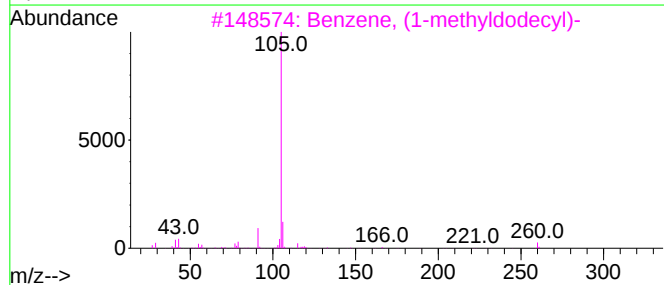
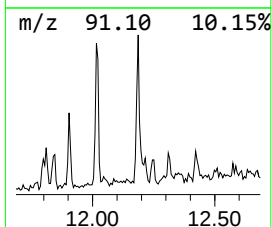
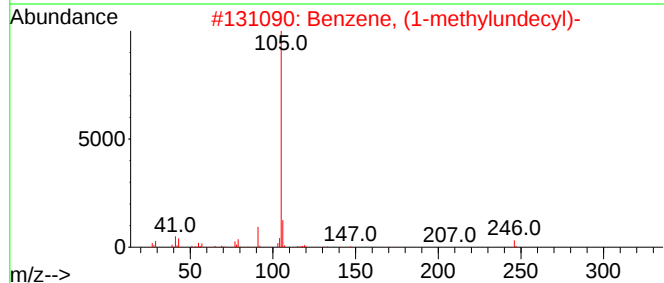
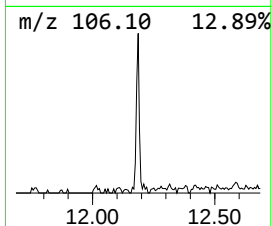
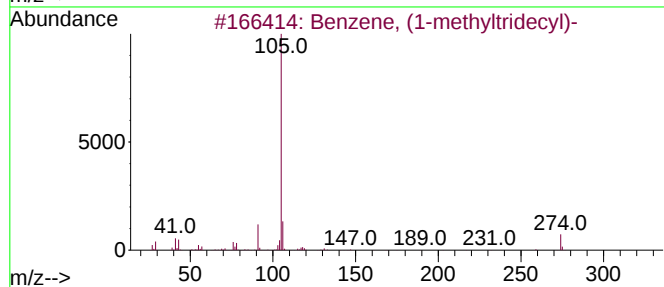
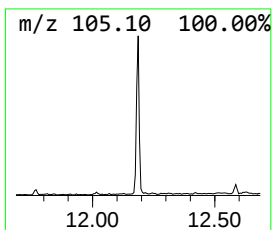
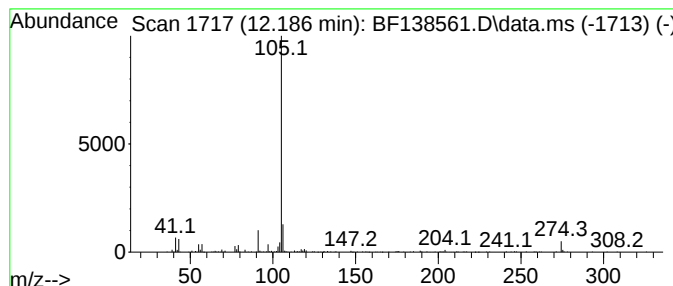
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzene, (1-methyltridecyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.186	4.06 ng	124217	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	74
2			Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	70
3			Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	53
4			Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	53
5			Benzene, (1-methylnonadecyl)-	358	C26H46	002398-66-5	53



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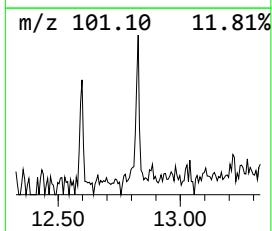
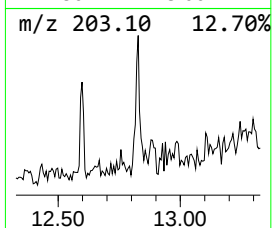
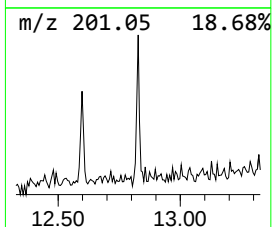
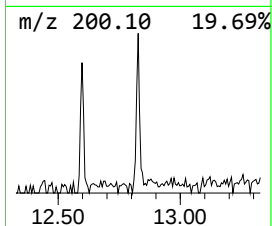
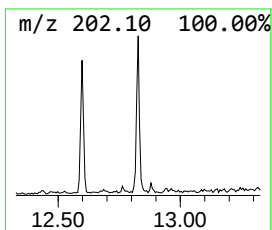
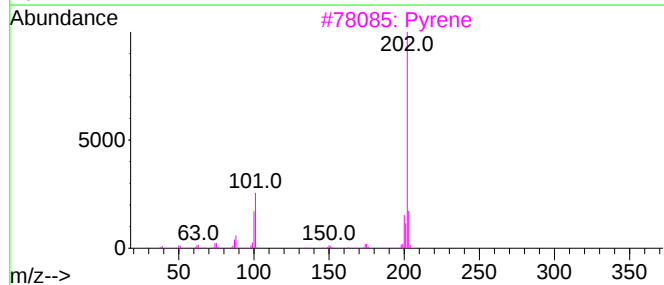
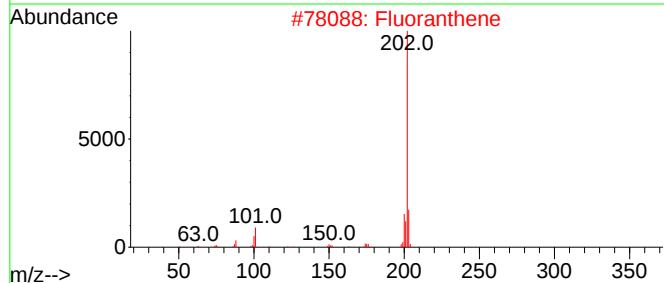
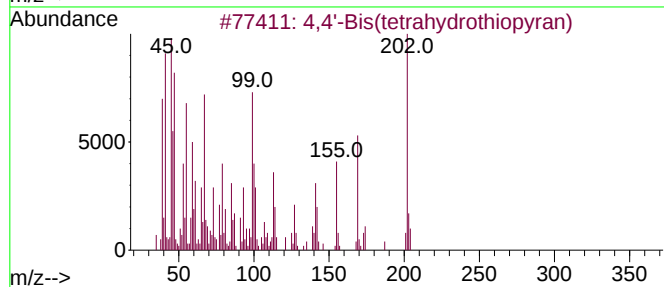
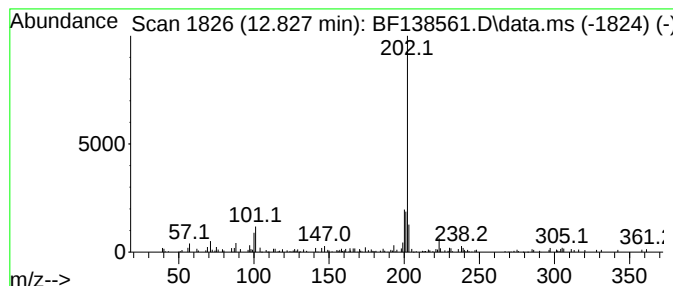
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.827	2.14 ng	51353	Chrysene-d12	14.021	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	60
2	Fluoranthene	202	C16H10	000206-44-0	58
3	Pyrene	202	C16H10	000129-00-0	58
4	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	53
5	1H-Pyrrol-3-amine, 5-(3-pyridiny...	202	C11H14N4	1000509-37-9	42



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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...	2.110	9.5	ng	235051	1	6.869	493300	20.0
unknown12.022	12.022	2.3	ng	71248	4	11.386	612139	20.0
Benzene, (1-met...	12.186	4.1	ng	124217	4	11.386	612139	20.0
4,4'-Bis(tetra...	12.827	2.1	ng	51353	5	14.021	480295	20.0