

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110824\
 Data File : BF140304.D
 Acq On : 08 Nov 2024 17:36
 Operator : RC/JU
 Sample : P4739-13 2X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-11

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-BF110524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140304.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	15	rVB	623353	718430	61.89%	4.933%
2	2.228	18	23	31	rVB2	8656	16332	1.41%	0.112%
3	3.946	308	315	329	rVB	11979	22045	1.90%	0.151%
4	5.081	504	508	515	rVB	36423	51936	4.47%	0.357%
5	5.487	567	577	589	rBV	764605	1011428	87.13%	6.945%
6	5.787	624	628	639	rVB	19890	31444	2.71%	0.216%
7	5.899	640	647	652	rBV3	13591	26088	2.25%	0.179%
8	5.946	652	655	663	rVV5	6995	13603	1.17%	0.093%
9	6.040	663	671	675	rVV4	16164	26775	2.31%	0.184%
10	6.128	680	686	692	rVV4	35292	72105	6.21%	0.495%
11	6.181	692	695	698	rVV	16808	21282	1.83%	0.146%
12	6.216	698	701	708	rVB6	6376	14011	1.21%	0.096%
13	6.316	713	718	721	rBV2	25014	39969	3.44%	0.274%
14	6.375	722	728	730	rVV3	16021	28070	2.42%	0.193%
15	6.404	730	733	741	rVV3	53119	99464	8.57%	0.683%
16	6.498	741	749	756	rVV	792225	1103800	95.09%	7.579%
17	6.557	756	759	765	rVV3	22051	41623	3.59%	0.286%
18	6.622	765	770	773	rVV3	21401	39232	3.38%	0.269%
19	6.657	774	776	779	rVV2	13060	14280	1.23%	0.098%
20	6.704	779	784	792	rVB2	141724	213826	18.42%	1.468%
21	6.840	797	807	808	rBV6	9297	23475	2.02%	0.161%
22	6.875	808	813	819	rVV	600344	763034	65.73%	5.239%
23	6.934	819	823	828	rVB	45809	55776	4.80%	0.383%
24	7.022	835	838	842	rVB3	15076	17628	1.52%	0.121%
25	7.146	853	859	863	rBV3	17501	24318	2.09%	0.167%
26	7.193	863	867	874	rVB3	14086	31806	2.74%	0.218%
27	7.263	874	879	885	rBV3	12858	21707	1.87%	0.149%
28	7.434	899	908	912	rBV	526185	671014	57.81%	4.608%
29	7.469	912	914	918	rVV	47530	50754	4.37%	0.349%
30	7.516	918	922	926	rVB4	10170	15186	1.31%	0.104%
31	7.687	947	951	959	rVB2	25551	37616	3.24%	0.258%
32	8.157	1024	1031	1038	rBV	732065	923556	79.56%	6.342%
33	8.369	1063	1067	1074	rBV5	8584	13997	1.21%	0.096%
34	8.575	1098	1102	1108	rBV	10397	14678	1.26%	0.101%
35	8.745	1127	1131	1136	rBV	18943	23226	2.00%	0.159%
36	8.869	1149	1152	1156	rVB	12067	13471	1.16%	0.092%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	9.175	1201	1204	1208	rVB2	11224	13376	1.15%	0.092%
38	9.228	1208	1213	1223	rBV	884010	1160815	100.00%	7.971%
39	9.310	1223	1227	1235	rVB2	24882	36895	3.18%	0.253%
40	9.498	1255	1259	1265	rBV	10724	16165	1.39%	0.111%
41	9.569	1267	1271	1274	rBV	13245	18903	1.63%	0.130%
42	9.634	1278	1282	1288	rVB3	17600	29116	2.51%	0.200%
43	9.692	1288	1292	1302	rVB7	6747	14837	1.28%	0.102%
44	9.775	1302	1306	1311	rBV	12665	16742	1.44%	0.115%
45	9.839	1312	1317	1321	rVB2	21554	30180	2.60%	0.207%
46	9.916	1324	1330	1334	rBV	704223	888261	76.52%	6.099%
47	10.116	1359	1364	1368	rBV3	13666	21581	1.86%	0.148%
48	10.163	1368	1372	1380	rVB5	10229	18167	1.57%	0.125%
49	10.339	1395	1402	1406	rBV3	25608	44120	3.80%	0.303%
50	10.463	1419	1423	1431	rVB4	10579	21072	1.82%	0.145%
51	10.563	1432	1440	1445	rBV3	19175	40626	3.50%	0.279%
52	10.628	1446	1451	1458	rVV	74504	101249	8.72%	0.695%
53	10.704	1459	1464	1476	rVV	417038	559314	48.18%	3.841%
54	10.828	1479	1485	1493	rVB2	42445	78882	6.80%	0.542%
55	11.139	1534	1538	1545	rBV8	14160	30060	2.59%	0.206%
56	11.269	1556	1560	1562	rBV	24156	33593	2.89%	0.231%
57	11.298	1562	1565	1571	rVB2	37274	52400	4.51%	0.360%
58	11.404	1578	1583	1592	rBV2	660996	967426	83.34%	6.643%
59	11.475	1592	1595	1599	rVB	27415	39734	3.42%	0.273%
60	11.692	1629	1632	1636	rBV2	24609	31344	2.70%	0.215%
61	11.739	1637	1640	1645	rVB2	17558	26272	2.26%	0.180%
62	11.863	1657	1661	1663	rBV4	22995	37105	3.20%	0.255%
63	11.928	1666	1672	1679	rVB3	118904	219442	18.90%	1.507%
64	12.016	1684	1687	1690	rBV2	37415	51223	4.41%	0.352%
65	12.104	1699	1702	1705	rBV2	32873	37767	3.25%	0.259%
66	12.457	1759	1762	1765	rBV	46389	65346	5.63%	0.449%
67	12.492	1765	1768	1774	rVB2	56785	80109	6.90%	0.550%
68	12.622	1786	1790	1794	rBV	227329	277317	23.89%	1.904%
69	12.851	1824	1829	1836	rBV	247880	423282	36.46%	2.906%
70	12.992	1848	1853	1861	rVB	840064	1093758	94.22%	7.510%
71	14.057	2029	2034	2045	rVB2	579300	971171	83.66%	6.669%
72	15.568	2287	2291	2304	rVB	324004	708881	61.07%	4.868%

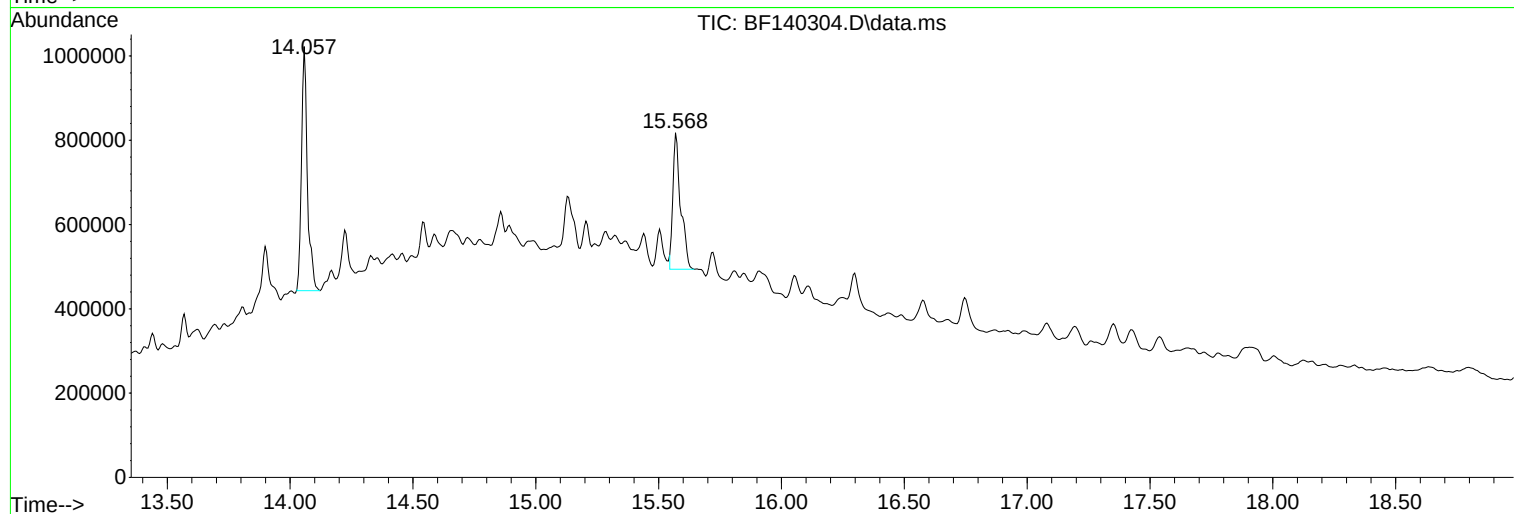
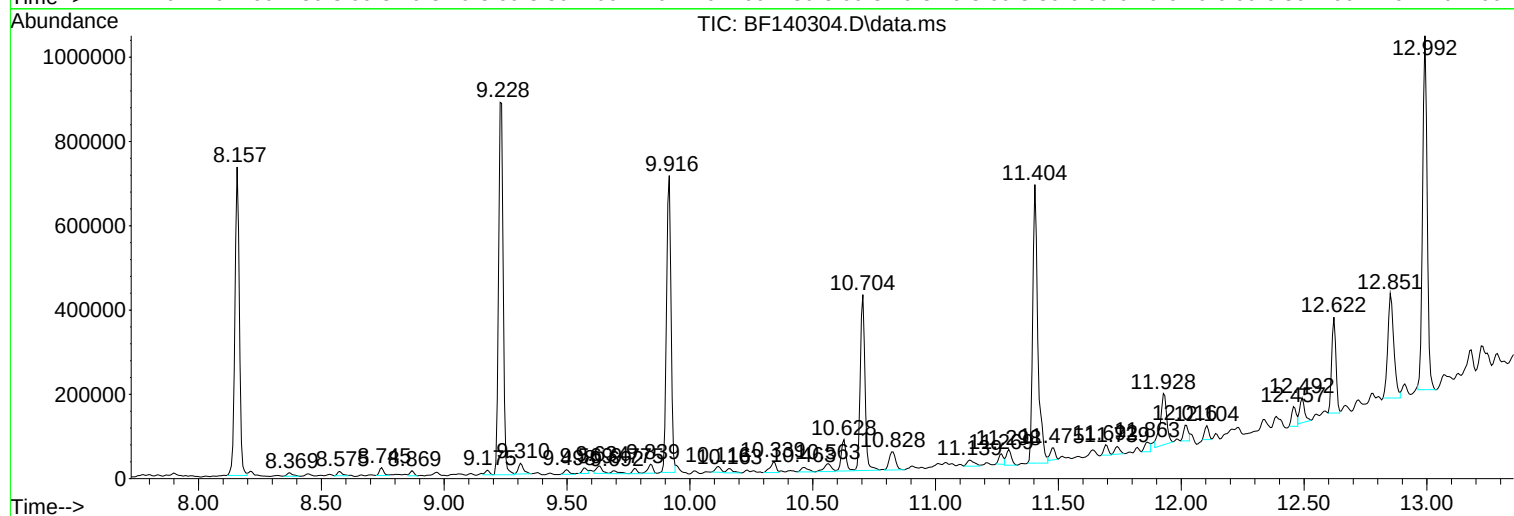
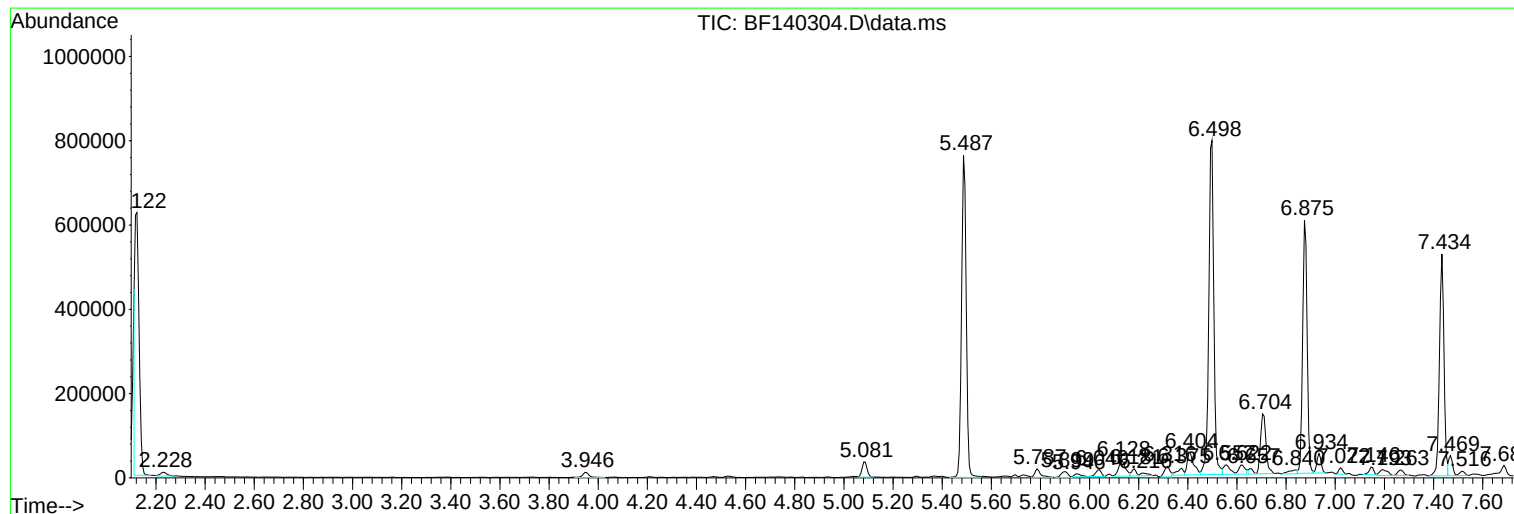
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF140304.D
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Operator : RC/JU
Sample : P4739-13 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11

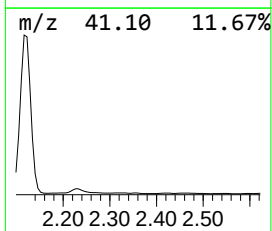
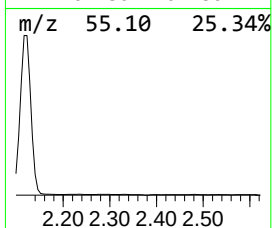
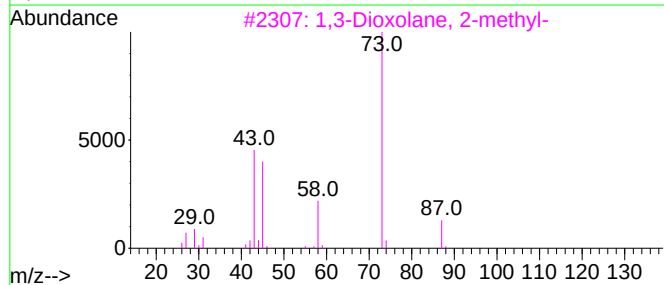
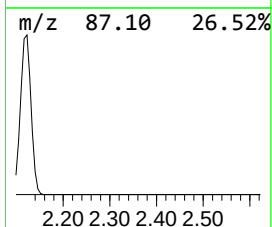
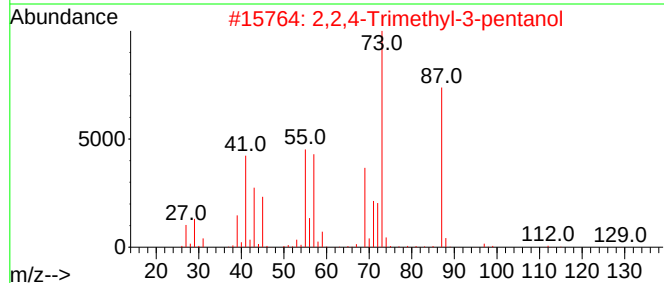
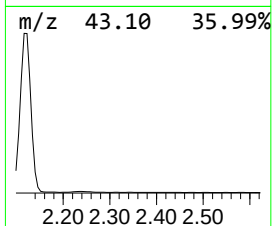
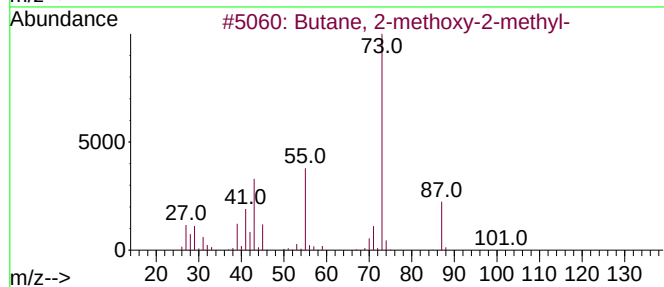
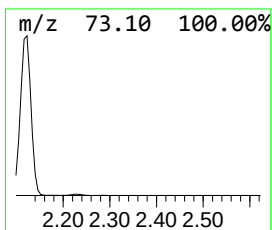
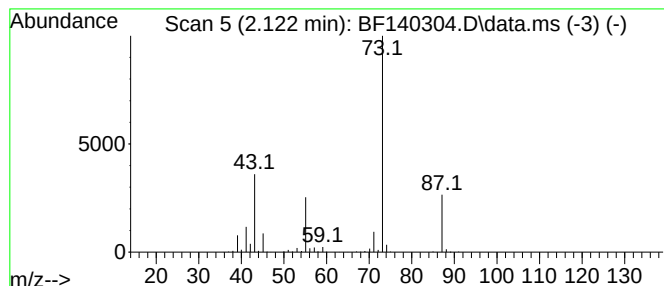
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.122	18.83 ng	718430	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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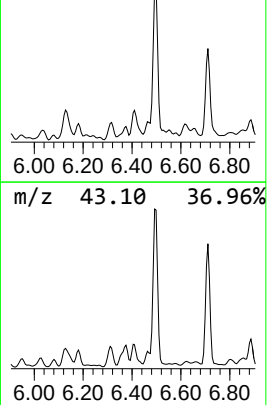
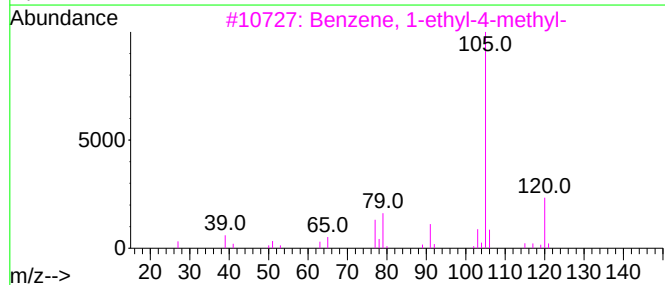
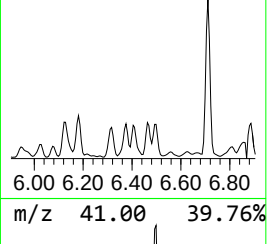
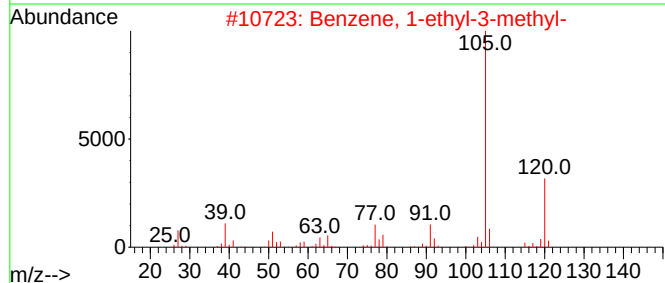
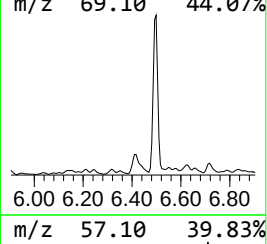
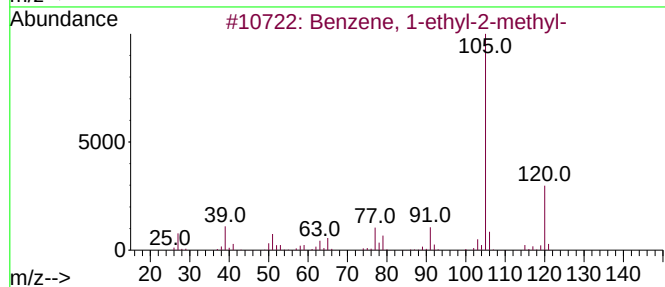
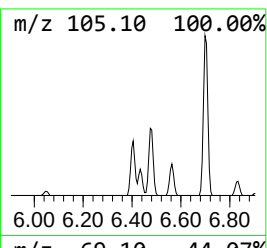
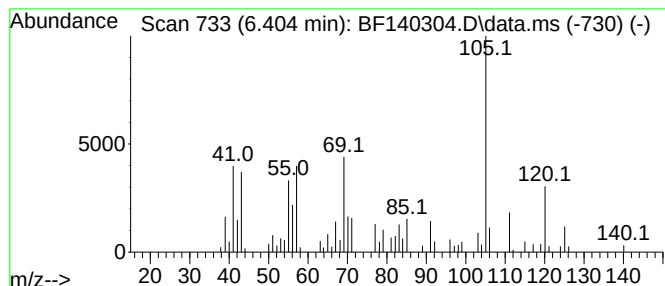
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.404	2.61 ng	99464	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	55
4			Mesitylene	120	C9H12	000108-67-8	50
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	45



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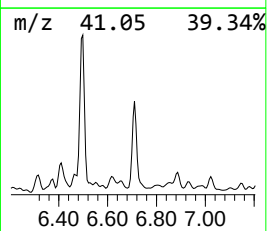
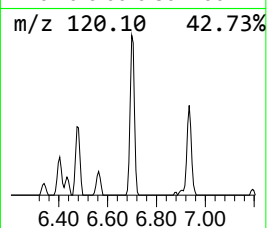
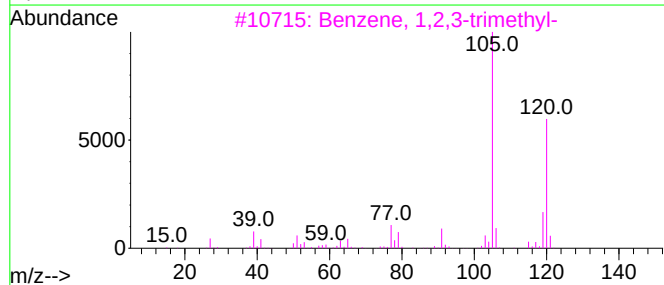
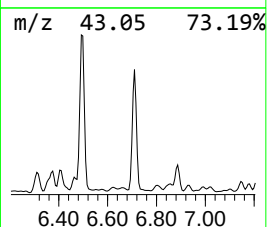
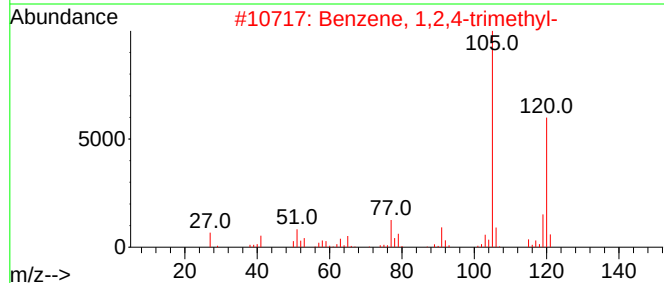
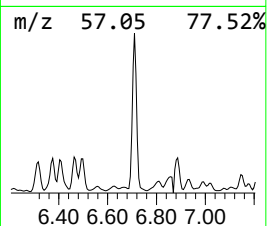
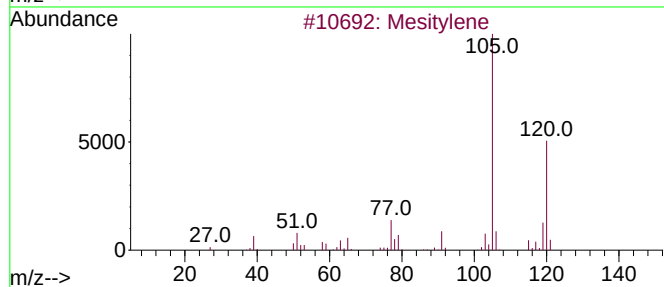
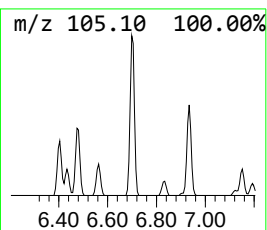
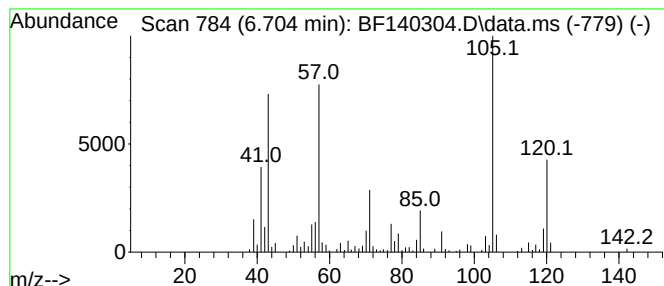
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Mesitylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	5.60 ng	213826	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	92
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	86
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	55
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	55



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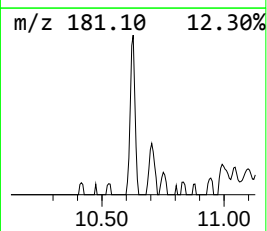
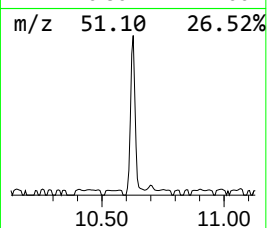
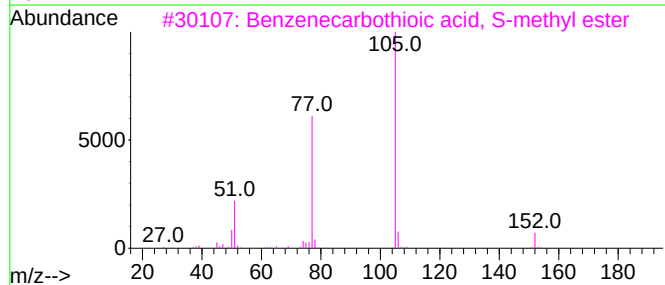
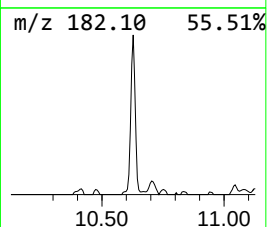
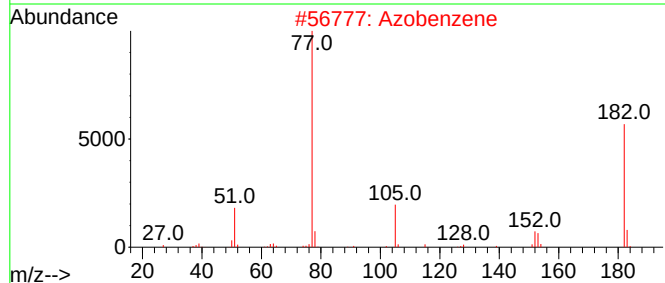
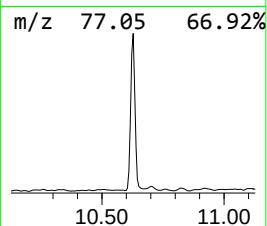
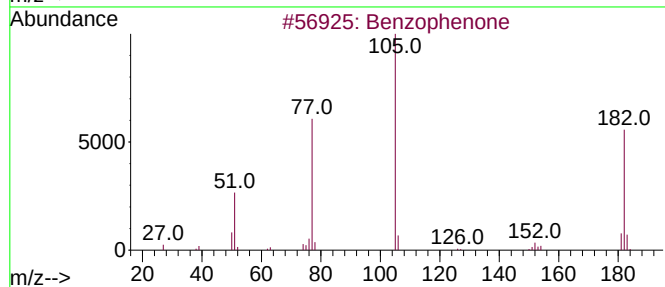
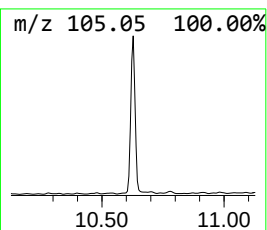
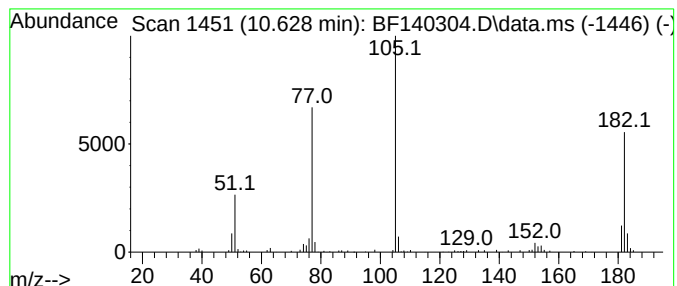
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	2.28 ng	101249	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	58
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110824\
Data File : BF140304.D
Acq On : 08 Nov 2024 17:36
Operator : RC/JU
Sample : P4739-13 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11

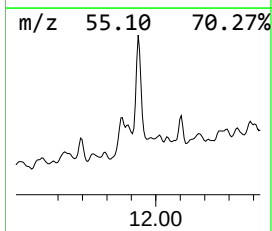
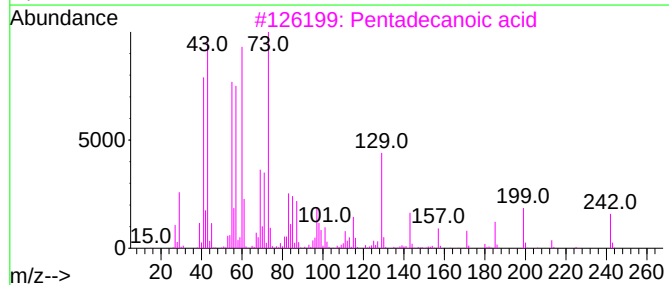
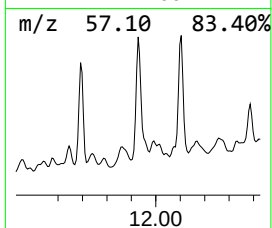
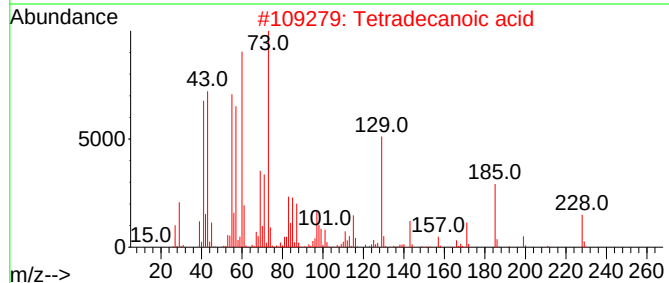
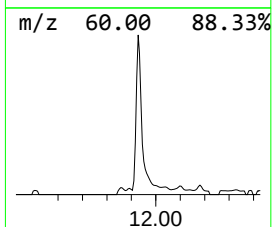
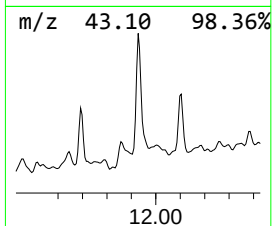
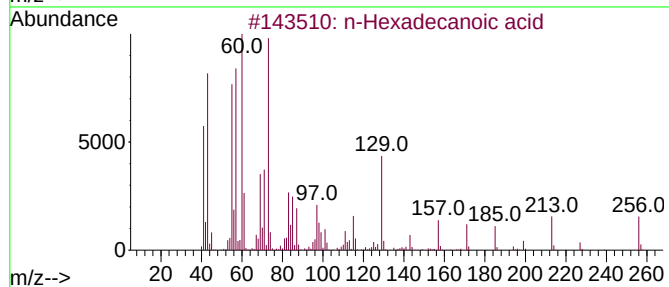
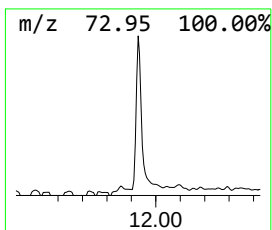
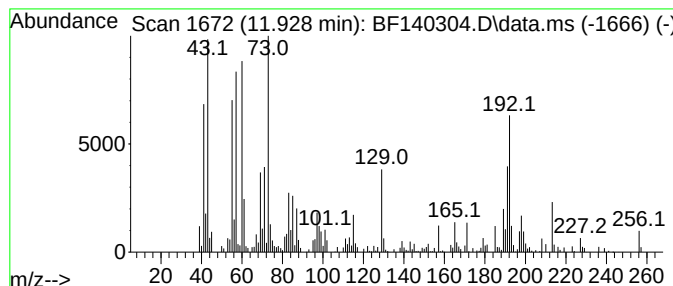
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	4.54 ng	219442	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Dodecanoic acid	200	C12H24O2	000143-07-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110824\
Data File : BF140304.D
Acq On : 08 Nov 2024 17:36
Operator : RC/JU
Sample : P4739-13 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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...	2.122	18.8	ng	718430	1	6.875	763034	20.0
Benzene, 1-ethy...	6.404	2.6	ng	99464	1	6.875	763034	20.0
Mesitylene	6.704	5.6	ng	213826	1	6.875	763034	20.0
Benzophenone	10.628	2.3	ng	101249	3	9.916	888261	20.0
n-Hexadecanoic ...	11.928	4.5	ng	219442	4	11.404	967426	20.0