

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
 Data File : BF141854.D
 Acq On : 05 Mar 2025 20:20
 Operator : RC/JU
 Sample : Q1489-05
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF022725.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.164	5	12	21	rVB	1086158	1738838	50.15%	5.649%
2	5.110	503	513	526	rBV2	27002	58329	1.68%	0.189%
3	5.499	573	579	584	rBV	2587696	3388657	97.74%	11.009%
4	6.499	743	749	762	rVB	2484026	3467024	100.00%	11.263%
5	6.887	810	815	820	rBV	759668	948038	27.34%	3.080%
6	7.440	903	909	914	rBV	1606809	2030639	58.57%	6.597%
7	7.693	948	952	958	rVB	74859	90430	2.61%	0.294%
8	8.163	1027	1032	1041	rBV	944607	1286667	37.11%	4.180%
9	8.375	1062	1068	1075	rVB3	34905	50994	1.47%	0.166%
10	8.875	1148	1153	1159	rBV2	37689	47015	1.36%	0.153%
11	9.240	1209	1215	1220	rBV	2506581	3252511	93.81%	10.566%
12	9.775	1302	1306	1311	rVB	38121	48634	1.40%	0.158%
13	9.916	1322	1330	1334	rBV	928141	1145217	33.03%	3.720%
14	9.951	1334	1336	1342	rVB	36401	37627	1.09%	0.122%
15	10.122	1359	1365	1369	rBV	41547	55684	1.61%	0.181%
16	10.463	1419	1423	1429	rVB	106861	132737	3.83%	0.431%
17	10.628	1446	1451	1458	rBV	210542	266885	7.70%	0.867%
18	10.698	1458	1463	1478	rBV	1484030	1941299	55.99%	6.307%
19	11.010	1508	1516	1519	rBV2	25677	44054	1.27%	0.143%
20	11.298	1561	1565	1570	rVB	32935	44917	1.30%	0.146%
21	11.404	1577	1583	1585	rBV	805253	1139517	32.87%	3.702%
22	11.475	1591	1595	1599	rBV	159062	190562	5.50%	0.619%
23	11.628	1616	1621	1628	rBV2	49383	92197	2.66%	0.300%
24	11.928	1664	1672	1677	rBV2	395989	635545	18.33%	2.065%
25	11.975	1678	1680	1683	rVV	46399	62547	1.80%	0.203%
26	12.016	1683	1687	1695	rVB2	117735	202404	5.84%	0.658%
27	12.198	1715	1718	1725	rVB	39761	56595	1.63%	0.184%
28	12.486	1764	1767	1773	rVB4	47200	85236	2.46%	0.277%
29	12.616	1784	1789	1793	rBV	598716	799004	23.05%	2.596%
30	12.657	1793	1796	1801	rVB2	62742	79017	2.28%	0.257%
31	12.710	1801	1805	1812	rBV	109452	171016	4.93%	0.556%
32	12.839	1821	1827	1833	rBV2	455177	667609	19.26%	2.169%
33	12.986	1847	1852	1858	rVB	2406319	3042804	87.76%	9.885%
34	13.169	1880	1883	1887	rVB	111543	131050	3.78%	0.426%
35	13.233	1891	1894	1898	rVB	85164	104534	3.02%	0.340%
36	13.880	2000	2004	2013	rVB	245140	391270	11.29%	1.271%

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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-BF022725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.033	2025	2030	2044	rBV2	957025	1751924	50.53%	5.691%
38	15.080	2204	2208	2217	rVB	173261	404770	11.67%	1.315%
39	15.510	2276	2281	2286	rBV	455604	698060	20.13%	2.268%

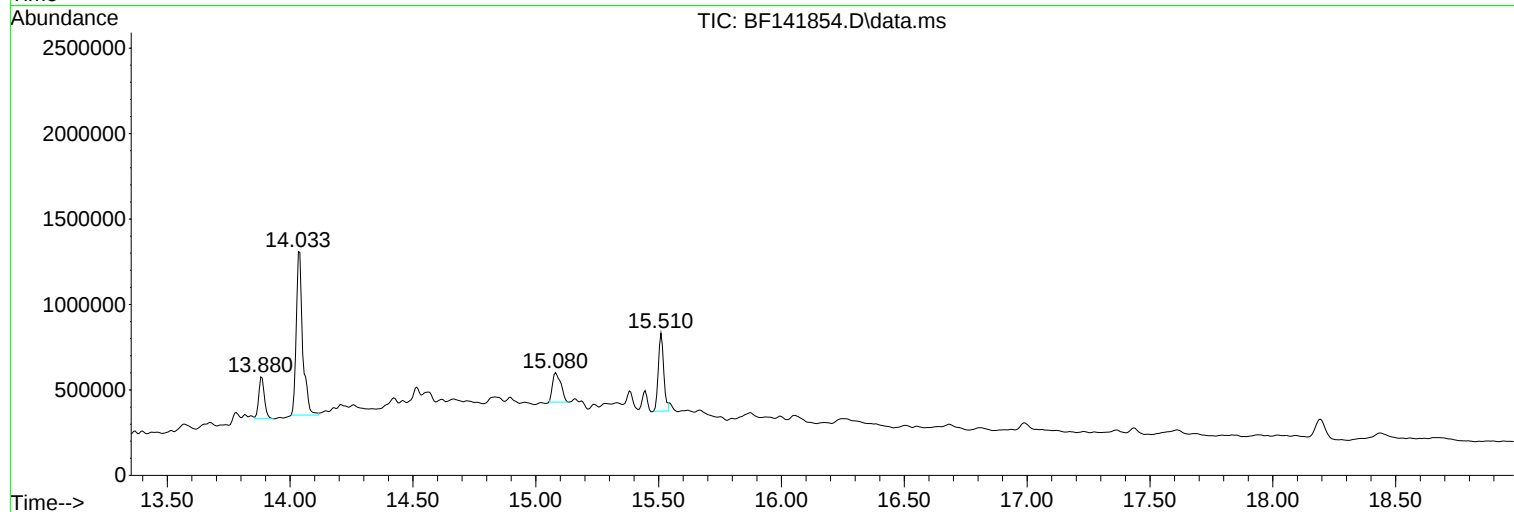
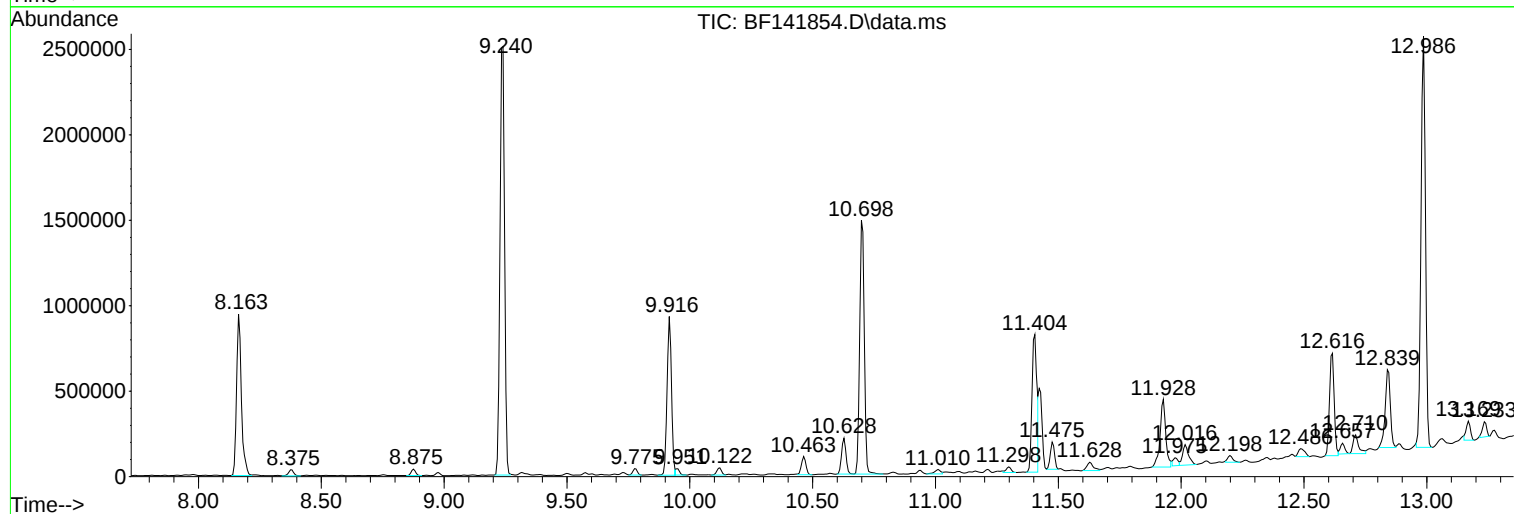
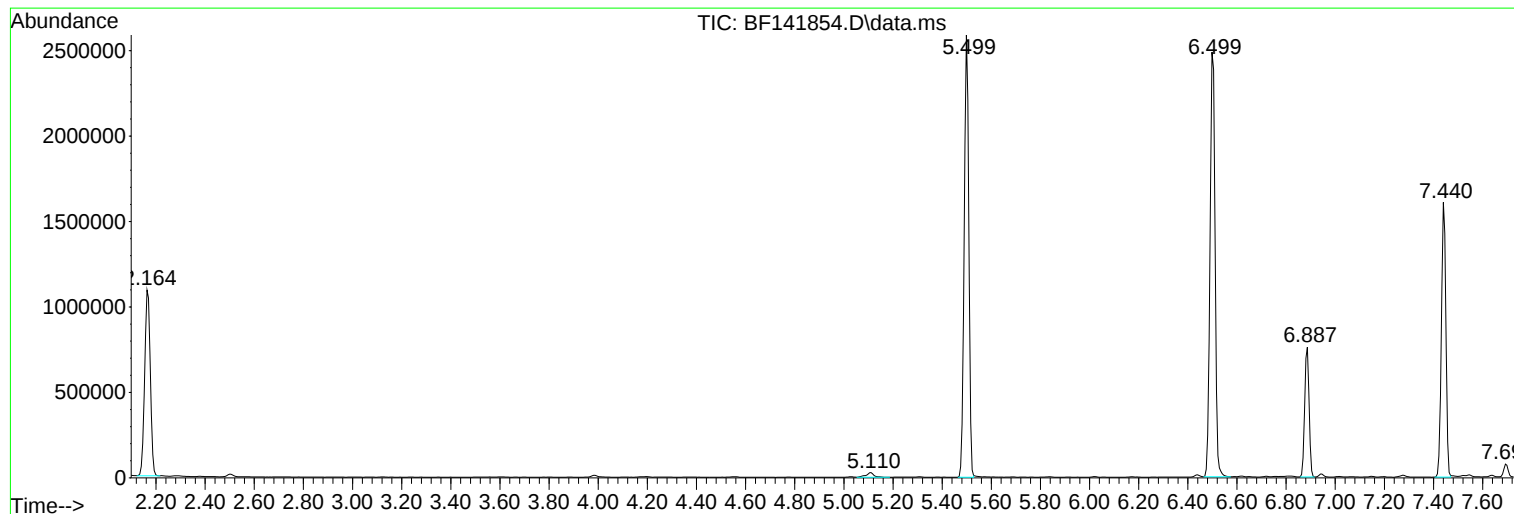
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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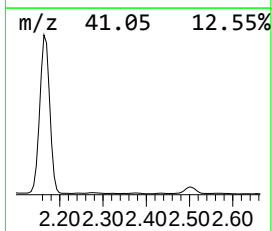
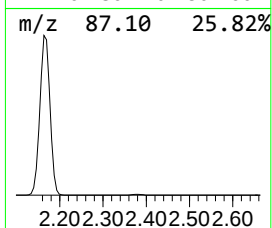
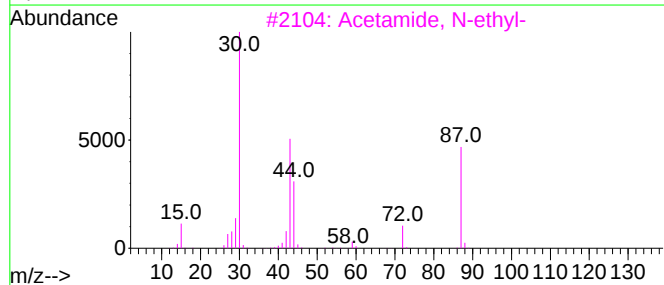
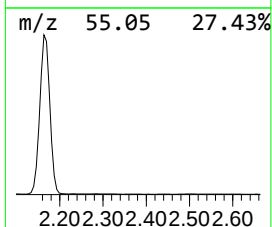
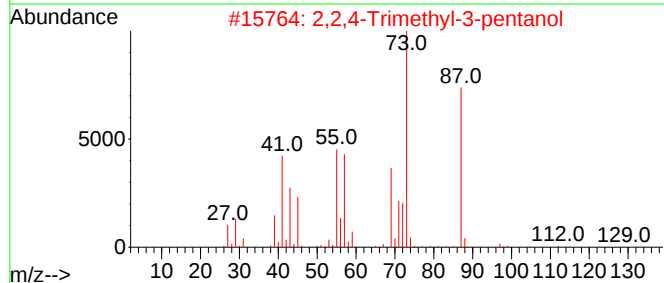
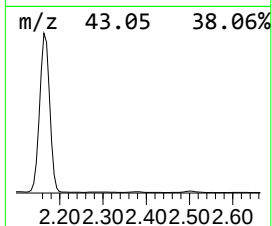
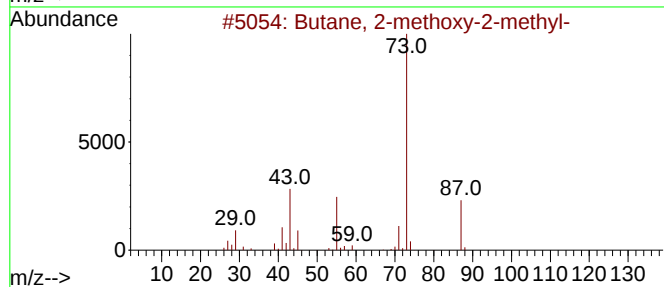
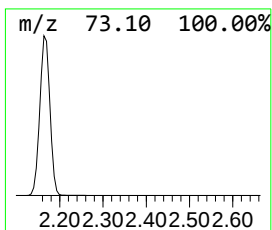
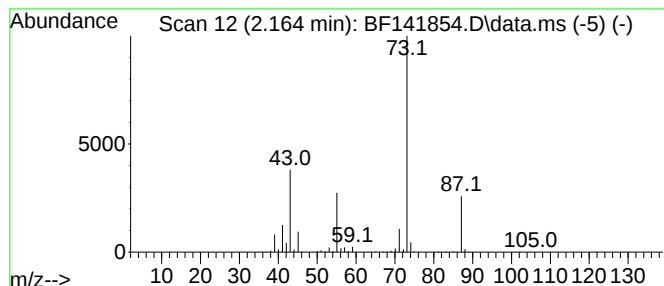
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.164	36.68 ng	1738840	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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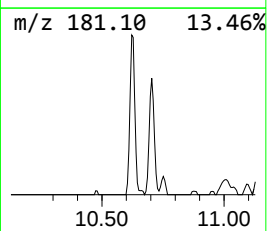
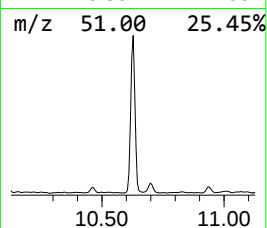
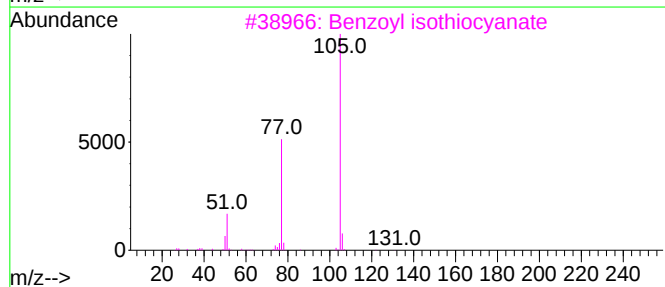
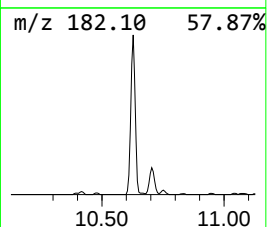
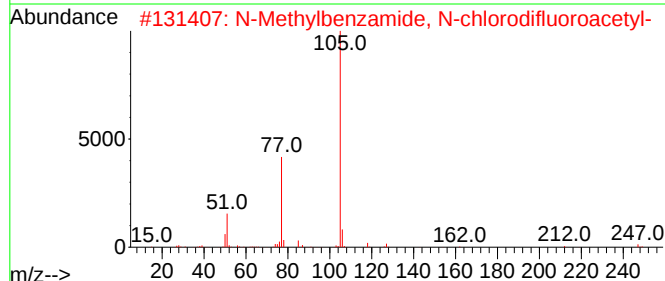
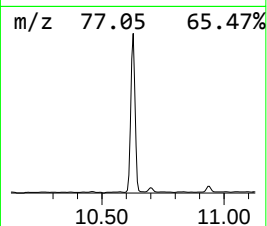
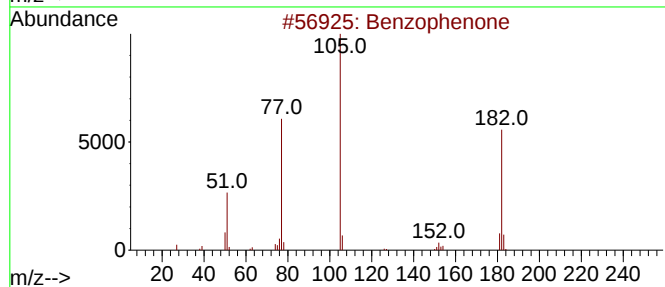
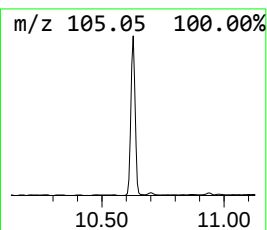
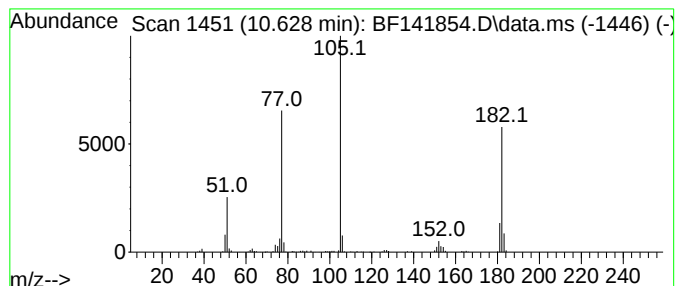
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	4.66 ng	266885	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47



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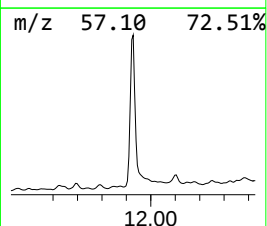
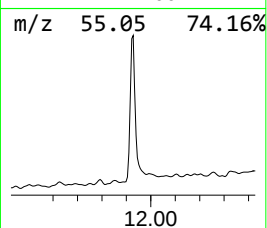
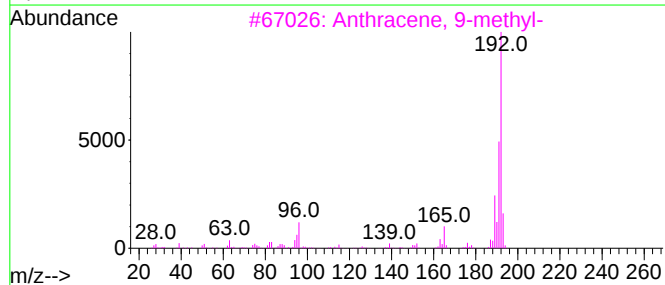
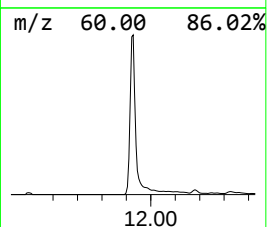
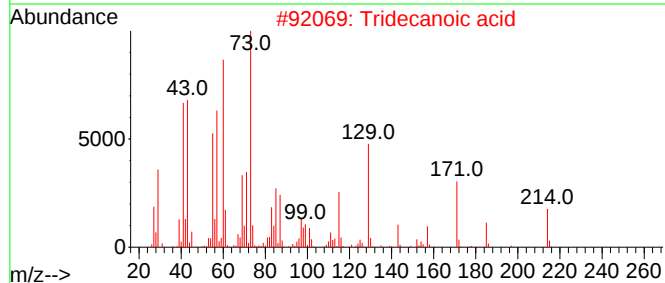
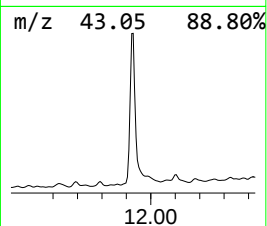
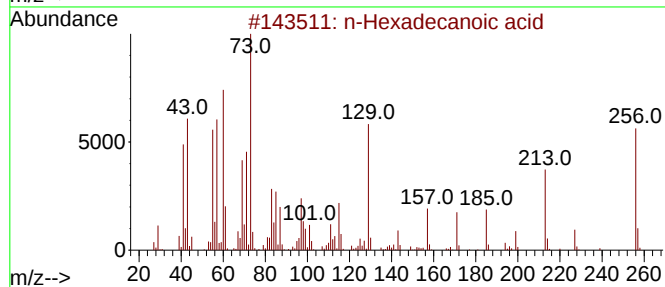
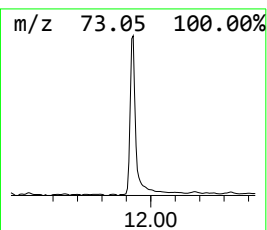
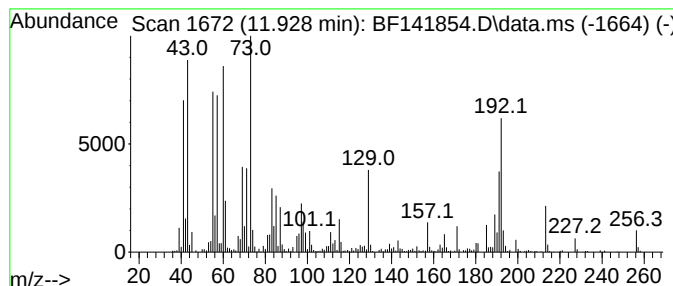
Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.928	11.15 ng	635545	Phenanthrene-d10		11.404	
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	91
3	Anthracene, 9-methyl-		192	C15H12	000779-02-2	90
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	86
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	83



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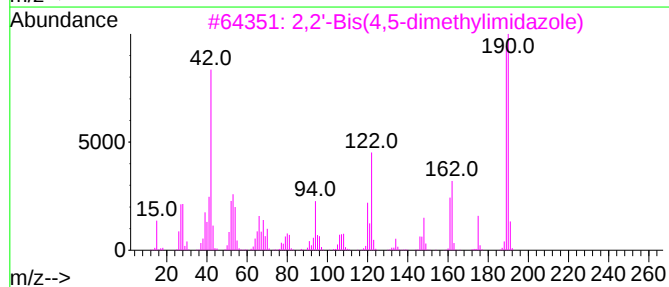
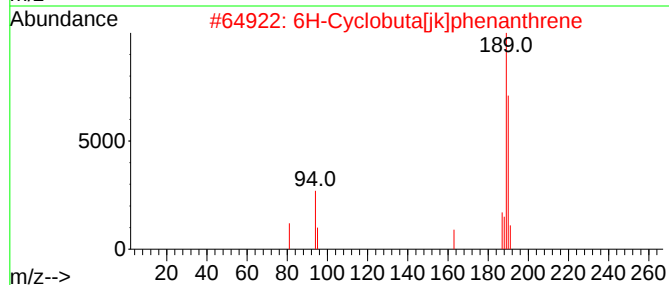
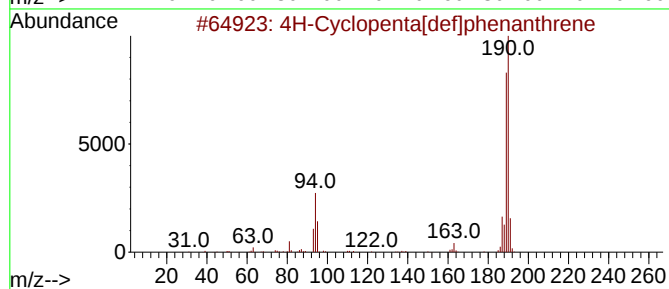
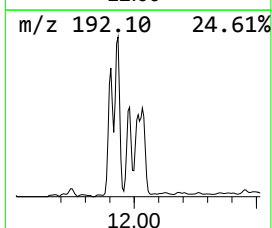
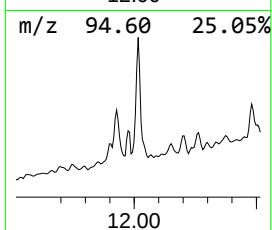
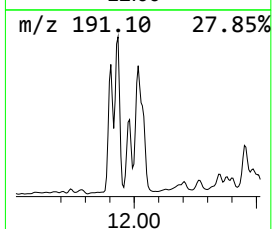
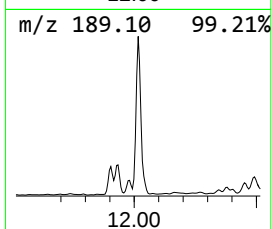
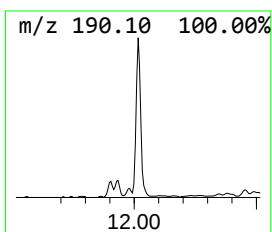
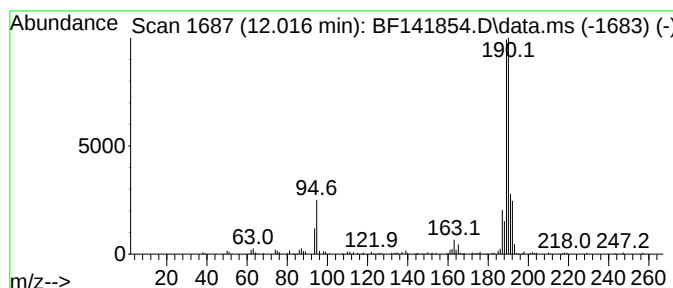
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	3.55 ng	202404	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
4			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25
5			1-Aminocyclopentanecarboxylic ac...	389	C20H36ClNO4	1000329-17-2	12



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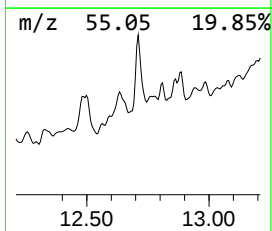
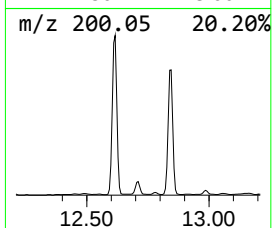
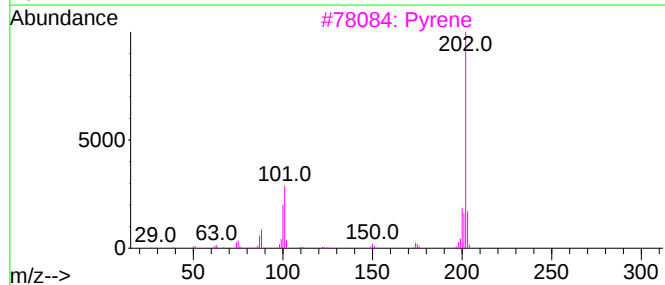
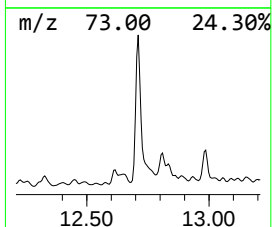
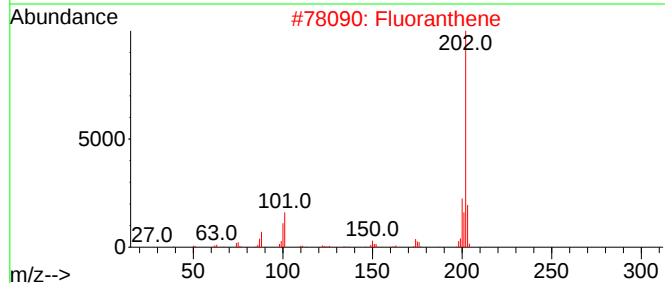
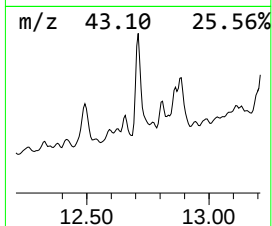
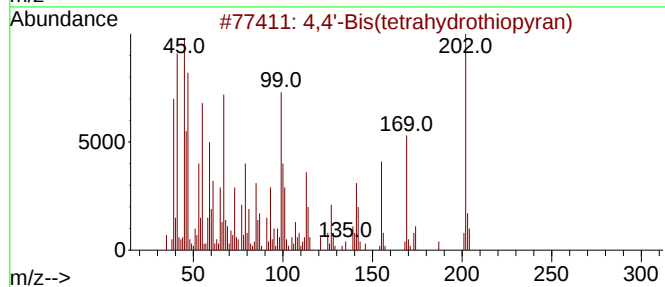
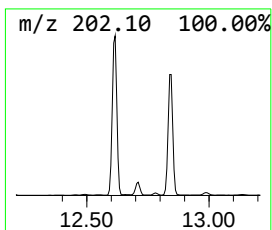
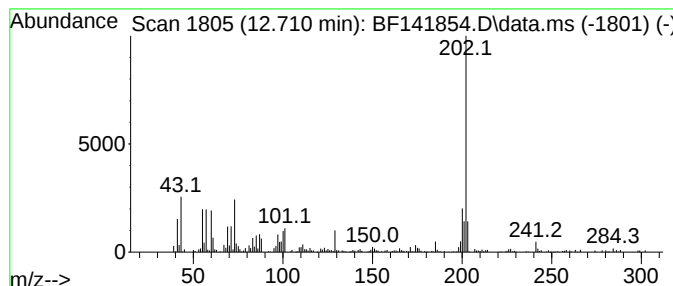
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	3.00 ng	171016	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	95
2			Fluoranthene	202	C16H10	000206-44-0	78
3			Pyrene	202	C16H10	000129-00-0	64
4			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	46
5			trans-2,4-Diamino-6-[1-propenyl]...	202	C9H10N6	040110-61-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141854.D
Acq On : 05 Mar 2025 20:20
Operator : RC/JU
Sample : Q1489-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

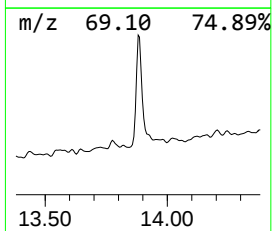
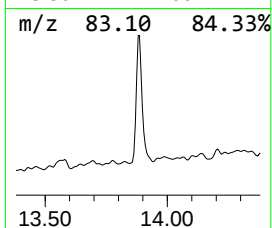
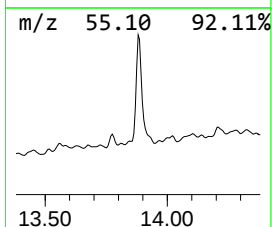
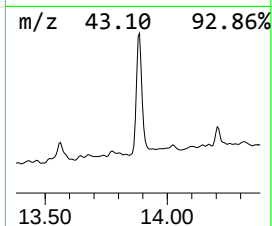
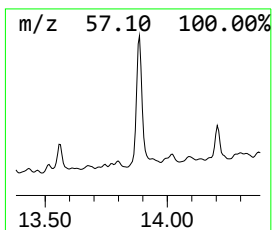
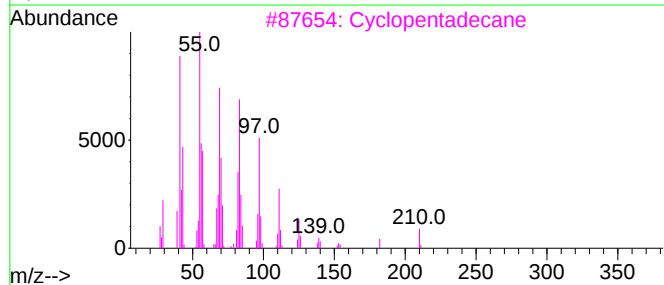
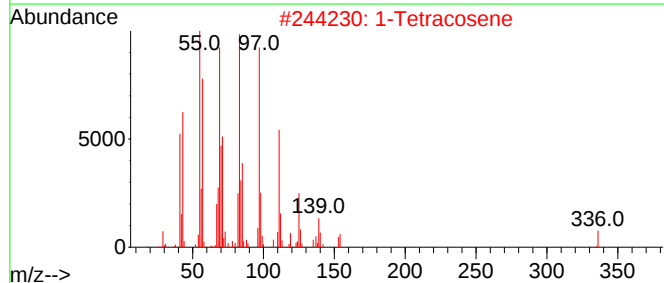
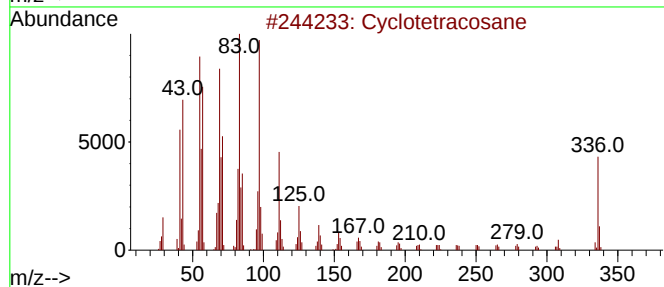
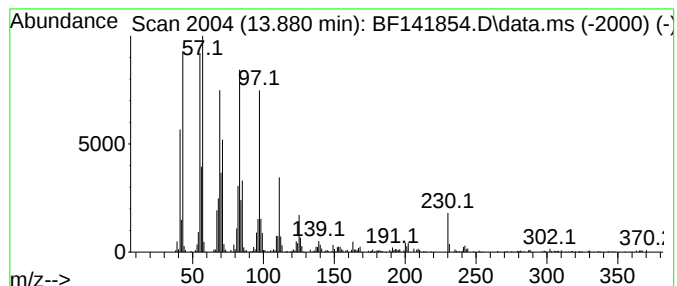
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.47 ng	391270	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	97
2			1-Tetracosene	336	C24H48	010192-32-2	97
3			Cyclopentadecane	210	C15H30	000295-48-7	96
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141854.D
Acq On : 05 Mar 2025 20:20
Operator : RC/JU
Sample : Q1489-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.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
Butane, 2-metho...	2.164	36.7	ng	1738840	1	6.887	948038	20.0
Benzophenone	10.628	4.7	ng	266885	3	9.916	1145220	20.0
n-Hexadecanoic ...	11.928	11.2	ng	635545	4	11.404	1139520	20.0
4H-Cyclopenta[d...]	12.016	3.5	ng	202404	4	11.404	1139520	20.0
4,4'-Bis(tetra...	12.710	3.0	ng	171016	4	11.404	1139520	20.0
Cyclotetracosane	13.880	4.5	ng	391270	5	14.039	1751920	20.0