

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
 Data File : BF136982.D
 Acq On : 05 Jan 2024 18:29
 Operator : CG\JU
 Sample : 06015-01 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-317-0-2

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.375	45	49	55	rVB4	5935	9908	1.16%	0.112%
2	5.016	494	498	509	rBV	28685	35325	4.12%	0.400%
3	5.428	565	568	581	rBV	767971	705252	82.21%	7.979%
4	6.434	735	739	756	rBV	752748	678129	79.05%	7.672%
5	6.781	795	798	802	rBV	420312	351354	40.96%	3.975%
6	7.345	890	894	903	rBV	513742	434581	50.66%	4.917%
7	8.057	1012	1015	1019	rBV	447682	409601	47.75%	4.634%
8	9.134	1195	1198	1202	rBV	939983	803196	93.63%	9.087%
9	9.675	1287	1290	1295	rBV	20549	19459	2.27%	0.220%
10	9.816	1310	1314	1318	rBV	512572	397633	46.35%	4.499%
11	9.845	1318	1319	1324	rVB	15827	13164	1.53%	0.149%
12	10.369	1405	1408	1413	rVB	12690	12441	1.45%	0.141%
13	10.610	1445	1449	1462	rBV	491800	433314	50.51%	4.902%
14	11.310	1564	1568	1570	rBV	509512	413531	48.21%	4.679%
15	11.333	1570	1572	1576	rVV	199563	151315	17.64%	1.712%
16	11.386	1578	1581	1584	rVB	41568	34315	4.00%	0.388%
17	11.551	1602	1609	1613	rBV2	15807	20130	2.35%	0.228%
18	11.816	1650	1654	1656	rBV	32897	32690	3.81%	0.370%
19	11.845	1656	1659	1665	rVV	100642	118665	13.83%	1.343%
20	11.892	1665	1667	1669	rVV	15276	14766	1.72%	0.167%
21	11.927	1669	1673	1675	rVV	40179	42853	5.00%	0.485%
22	11.951	1675	1677	1683	rVB	19063	16550	1.93%	0.187%
23	12.110	1702	1704	1707	rVB	16662	12920	1.51%	0.146%
24	12.145	1707	1710	1714	rVB	15697	15139	1.76%	0.171%
25	12.263	1725	1730	1733	rBV4	8570	9705	1.13%	0.110%
26	12.369	1743	1748	1750	rBV	18926	21498	2.51%	0.243%
27	12.404	1750	1754	1756	rVV4	13805	17410	2.03%	0.197%
28	12.457	1760	1763	1768	rVB2	17217	20672	2.41%	0.234%
29	12.533	1770	1776	1779	rBV	253993	253110	29.51%	2.864%
30	12.633	1789	1793	1796	rBV2	22855	26961	3.14%	0.305%
31	12.763	1809	1815	1820	rVB	257539	252765	29.47%	2.860%
32	12.810	1820	1823	1830	rBV4	26359	35920	4.19%	0.406%
33	12.904	1835	1839	1845	rVB	991694	857817	100.00%	9.705%
34	12.980	1848	1852	1856	rVV2	15249	21105	2.46%	0.239%
35	13.092	1864	1871	1875	rBV	37058	59736	6.96%	0.676%
36	13.133	1875	1878	1880	rBV4	14738	14647	1.71%	0.166%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
 Data File : BF136982.D
 Acq On : 05 Jan 2024 18:29
 Operator : CG\JU
 Sample : 06015-01 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-317-0-2

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.157	1880	1882	1885	rBV	22168	18002	2.10%	0.204%
38	13.198	1885	1889	1893	rBV2	26900	35846	4.18%	0.406%
39	13.292	1902	1905	1907	rBV	19500	18117	2.11%	0.205%
40	13.321	1907	1910	1913	rBV2	21197	22162	2.58%	0.251%
41	13.604	1956	1958	1963	rBV	27258	33703	3.93%	0.381%
42	13.716	1974	1977	1979	rBV	30153	28458	3.32%	0.322%
43	13.739	1979	1981	1984	rVB	21141	17724	2.07%	0.201%
44	13.769	1984	1986	1987	rBV	13269	9940	1.16%	0.112%
45	13.816	1991	1994	1996	rBV2	27555	27059	3.15%	0.306%
46	13.968	2015	2020	2023	rBV2	551350	604680	70.49%	6.841%
47	13.992	2023	2024	2030	rVV	118350	93709	10.92%	1.060%
48	14.063	2033	2036	2040	rVB2	34371	47542	5.54%	0.538%
49	14.127	2044	2047	2050	rBV4	18029	26411	3.08%	0.299%
50	14.363	2084	2087	2089	rVB	22166	20952	2.44%	0.237%
51	14.745	2150	2152	2155	rVB2	25014	18740	2.18%	0.212%
52	14.892	2175	2177	2180	rVB3	33340	27364	3.19%	0.310%
53	15.021	2195	2199	2202	rBV	99282	146991	17.14%	1.663%
54	15.086	2207	2210	2214	rBV2	52573	61171	7.13%	0.692%
55	15.327	2248	2251	2258	rVB	63737	81892	9.55%	0.927%
56	15.392	2258	2262	2267	rVB	84944	110402	12.87%	1.249%
57	15.457	2268	2273	2285	rVV2	296229	471093	54.92%	5.330%
58	15.921	2349	2352	2358	rVB	54955	83694	9.76%	0.947%
59	16.974	2527	2531	2537	rVB3	33421	65449	7.63%	0.740%

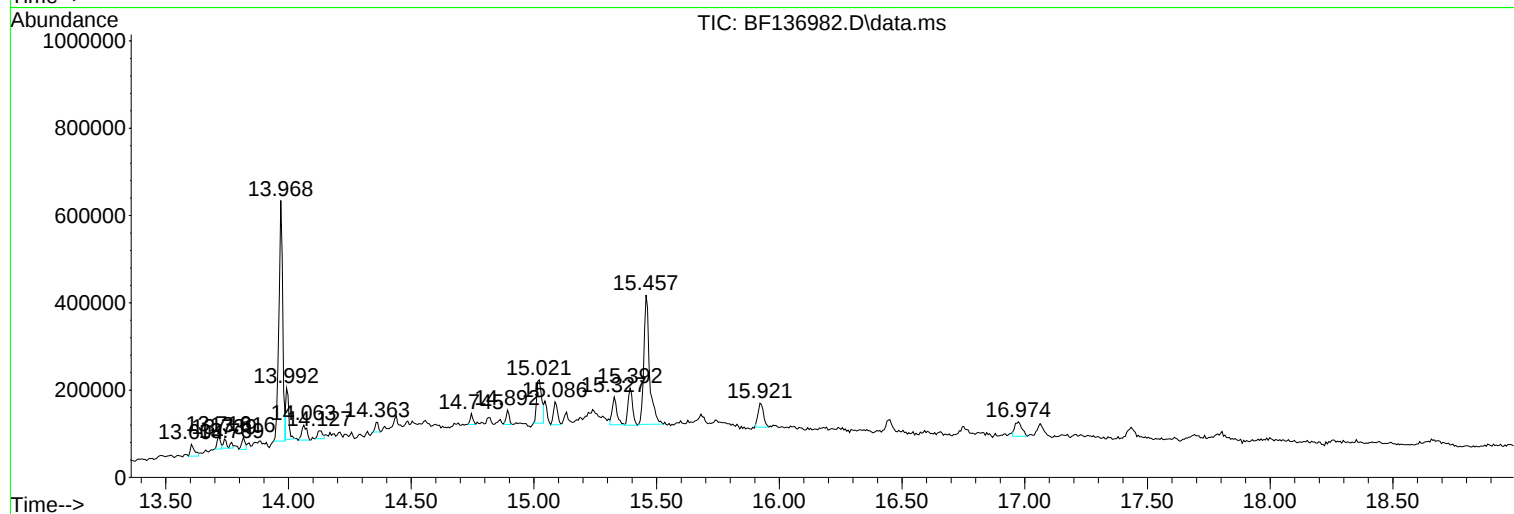
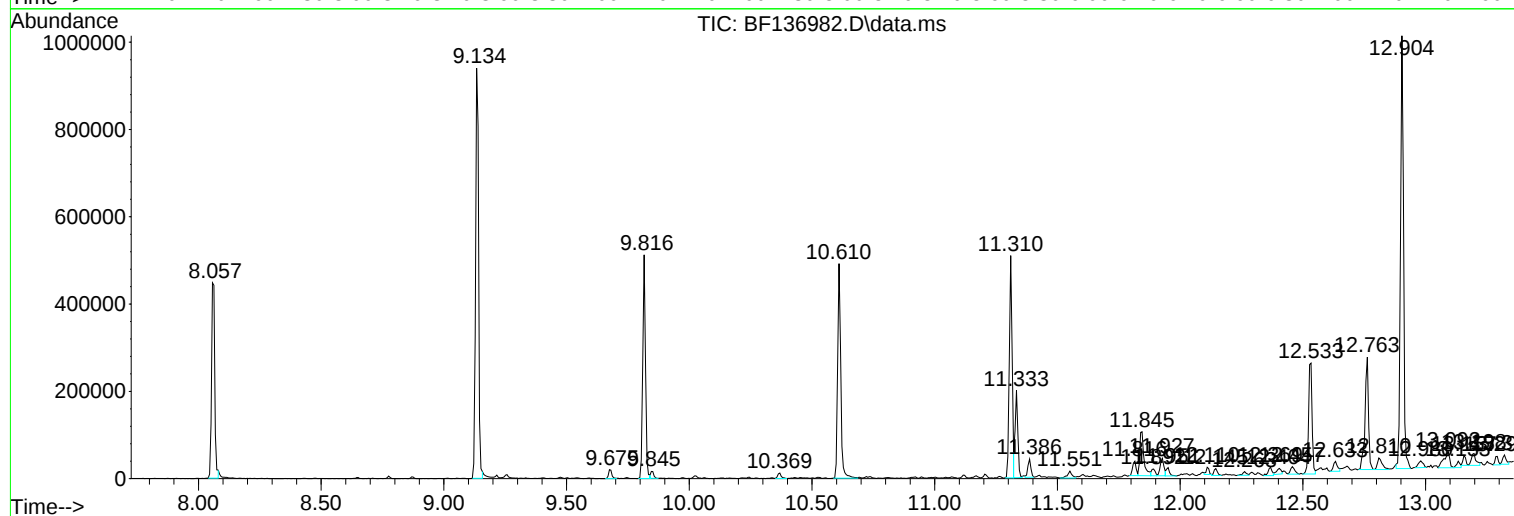
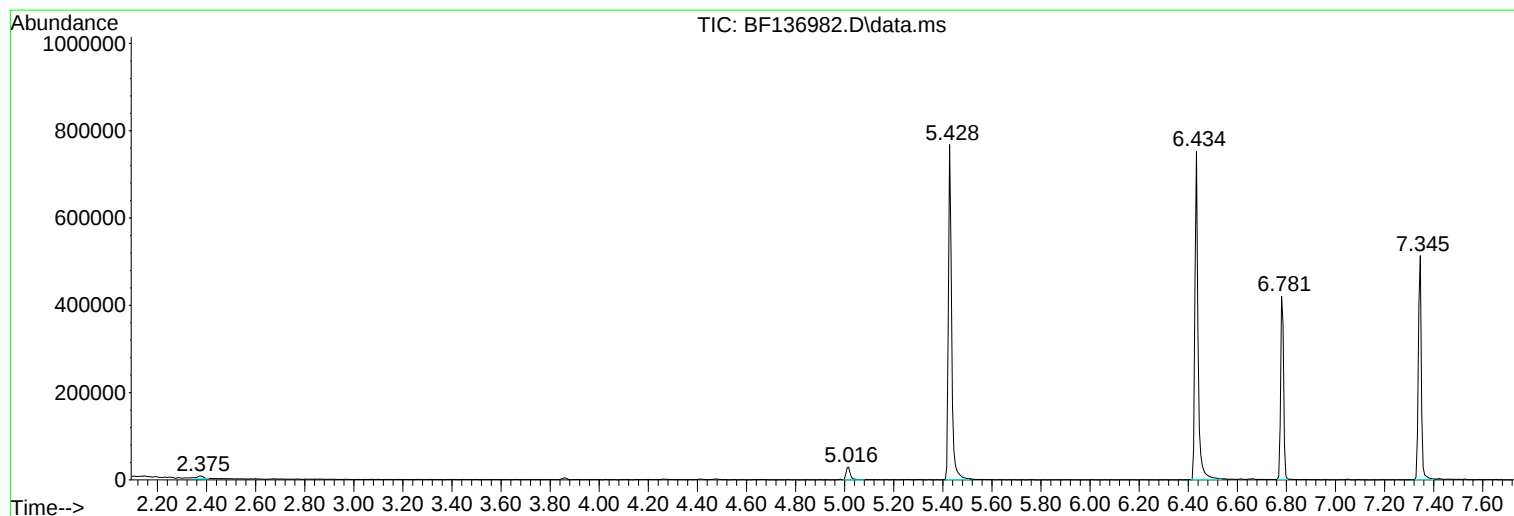
Sum of corrected areas: 8838678

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136982.D
Acq On : 05 Jan 2024 18:29
Operator : CG\JU
Sample : 06015-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136982.D
Acq On : 05 Jan 2024 18:29
Operator : CG\JU
Sample : 06015-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317-0-2

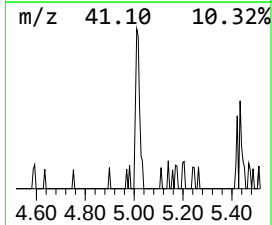
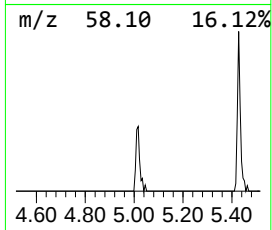
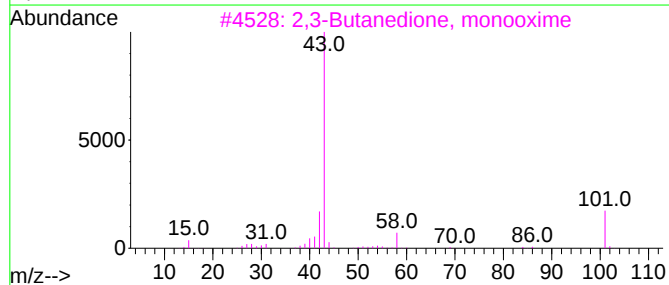
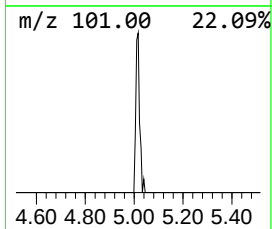
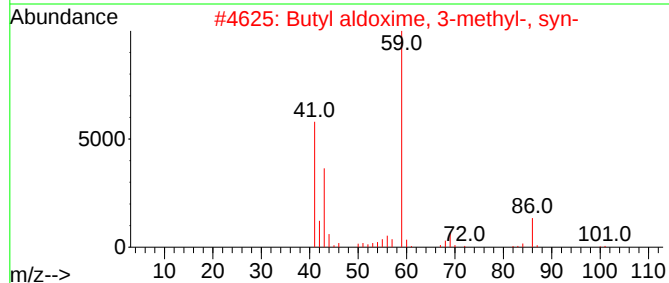
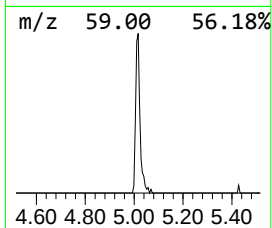
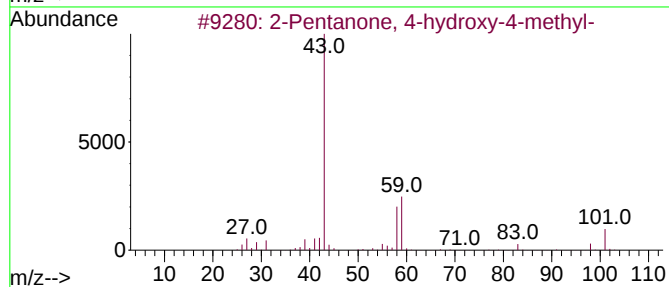
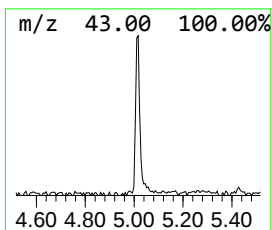
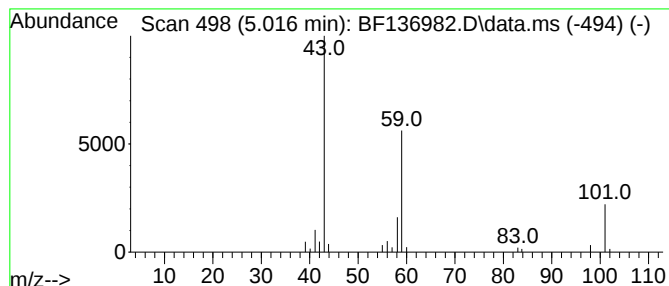
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.01 ng	35325	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136982.D
Acq On : 05 Jan 2024 18:29
Operator : CG\JU
Sample : 06015-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

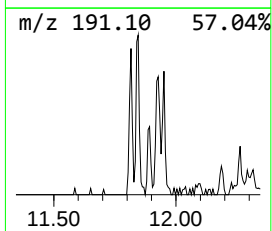
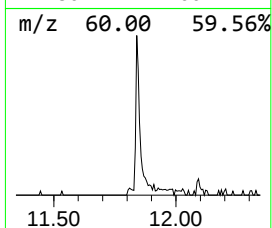
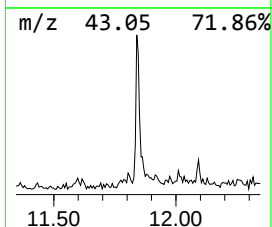
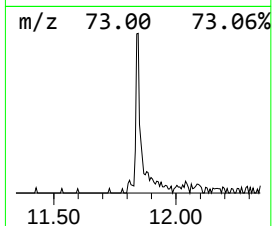
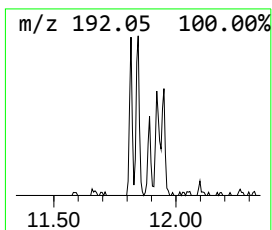
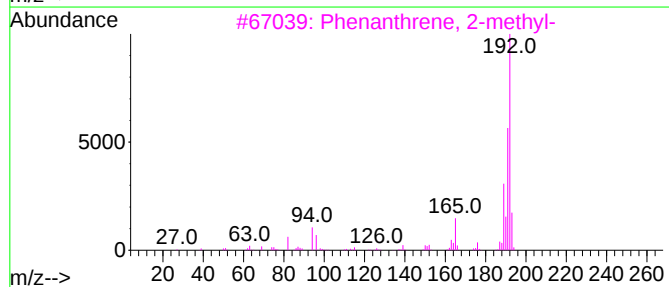
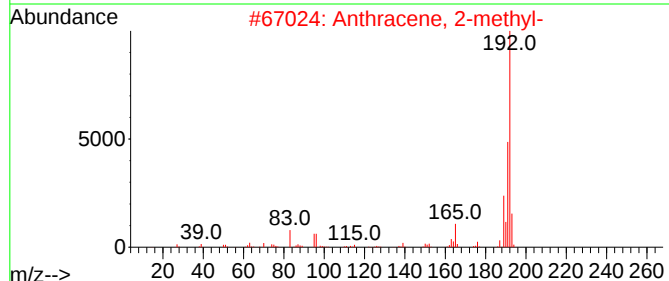
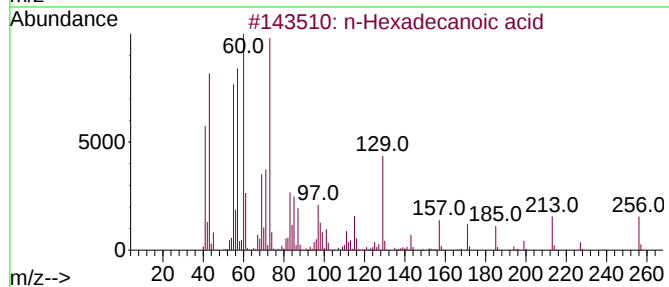
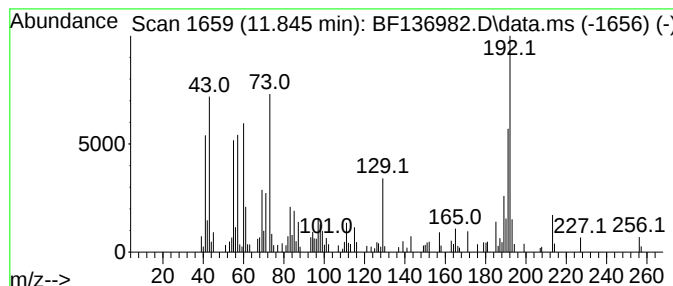
Instrument :
BNA_F
ClientSampleId :
MR-317-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.845	5.74 ng	118665	Phenanthrene-d10		11.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	95
2	Anthracene, 2-methyl-		192	C15H12	000613-12-7	86
3	Phenanthrene, 2-methyl-		192	C15H12	002531-84-2	86
4	Anthracene, 9-methyl-		192	C15H12	000779-02-2	60
5	Anthracene, 1-methyl-		192	C15H12	000610-48-0	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136982.D
Acq On : 05 Jan 2024 18:29
Operator : CG\JU
Sample : 06015-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

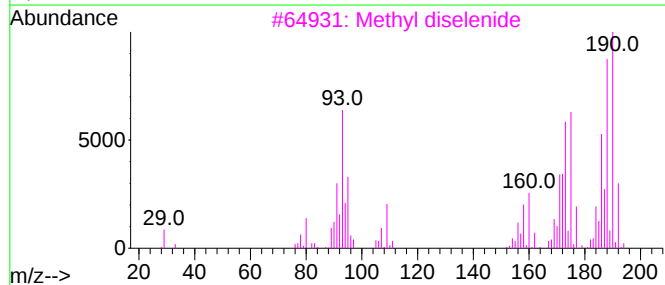
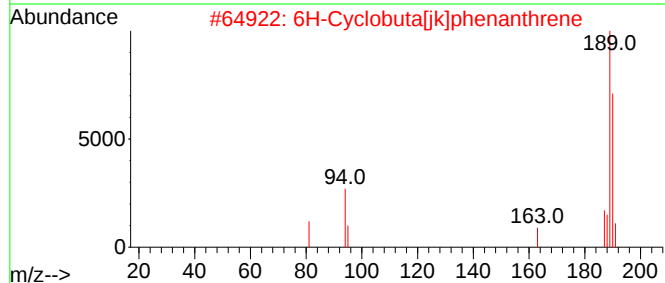
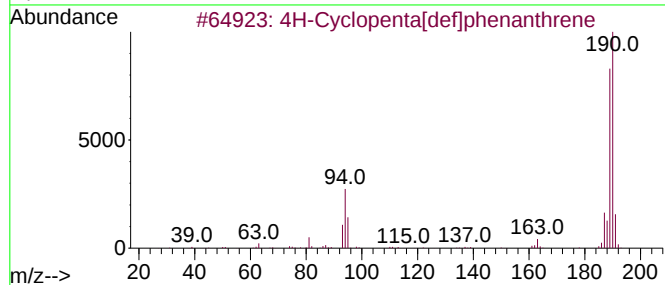
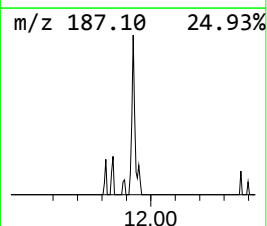
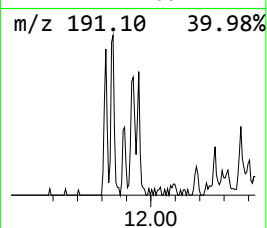
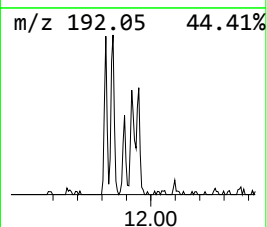
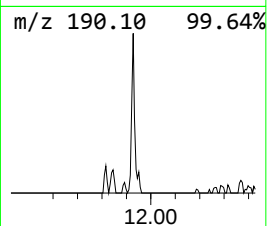
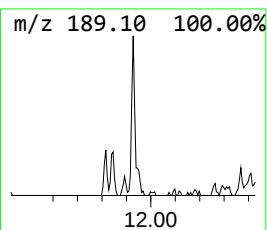
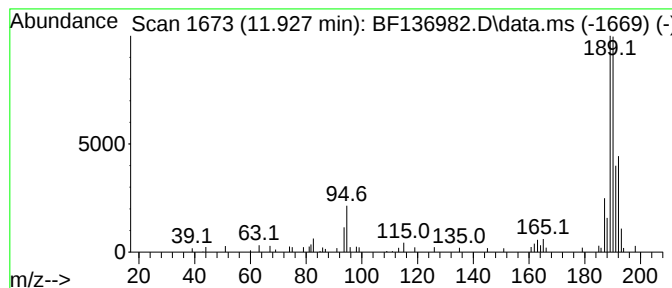
Instrument :
BNA_F
ClientSampleId :
MR-317-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.928	2.07 ng	42853	Phenanthrene-d10		11.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	62
2	6H-Cyclobuta[jk]phenanthrene		190	C15H10	083469-43-6	52
3	Methyl diselenide		190	C2H6Se2	007101-31-7	43
4	2,4(1H,3H)-Pyrimidinedione, 5-br...		190	C4H3BrN2O2	000051-20-7	38
5	2,2'-Bis(4,5-dimethylimidazole)		190	C10H14N4	069286-06-2	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136982.D
Acq On : 05 Jan 2024 18:29
Operator : CG\JU
Sample : 06015-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317-0-2

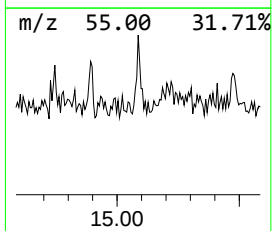
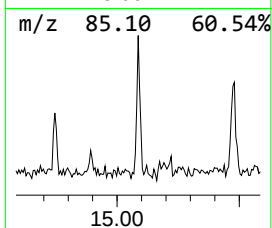
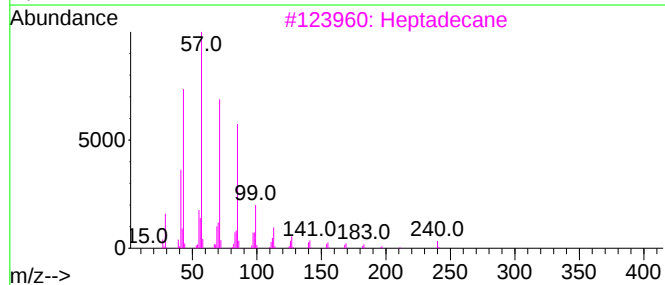
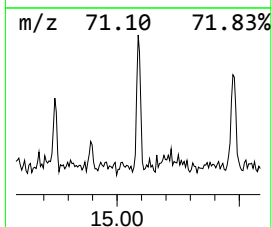
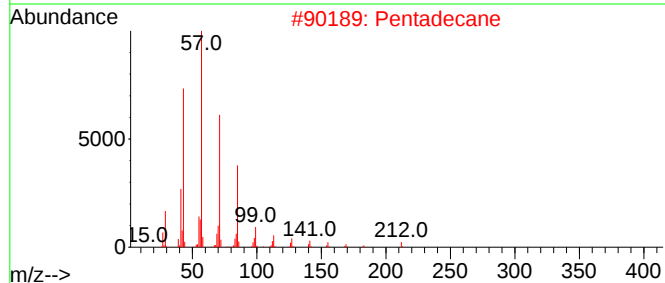
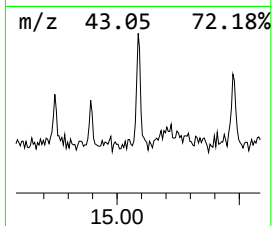
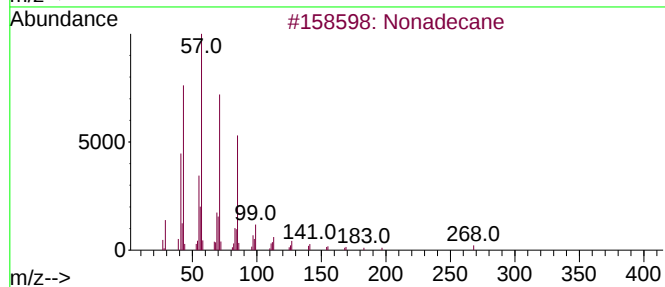
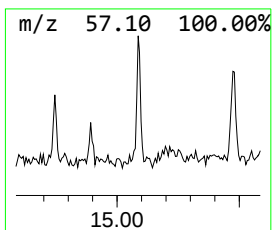
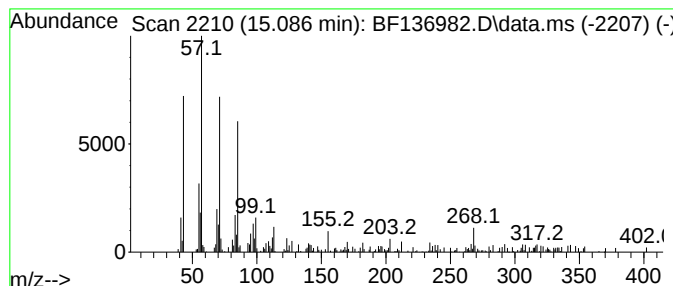
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	2.60 ng	61171	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Pentadecane	212	C15H32	000629-62-9	83
3			Heptadecane	240	C17H36	000629-78-7	64
4			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64
5			Hexacosane	366	C26H54	000630-01-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136982.D
Acq On : 05 Jan 2024 18:29
Operator : CG\JU
Sample : 06015-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317-0-2

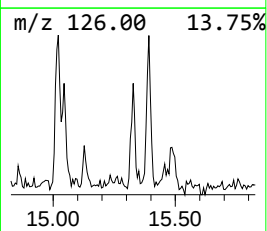
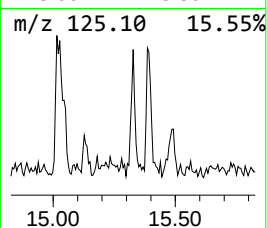
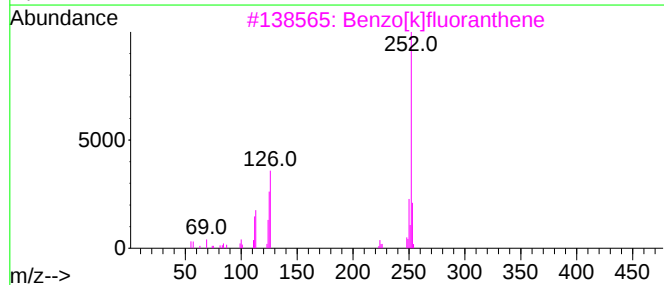
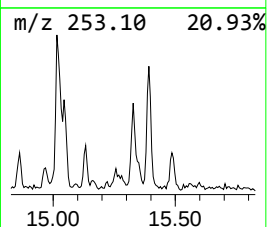
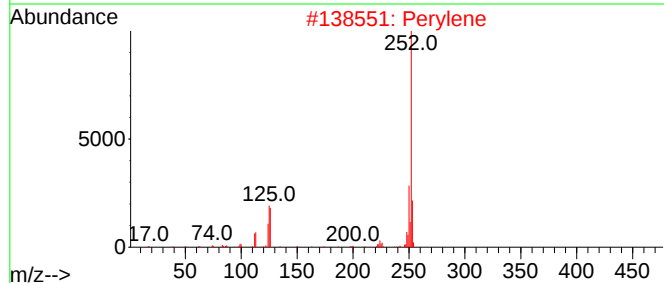
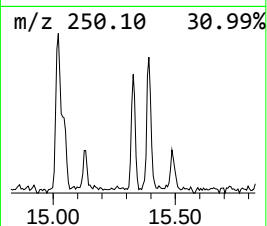
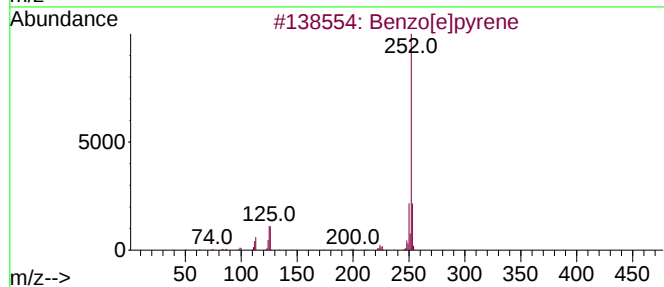
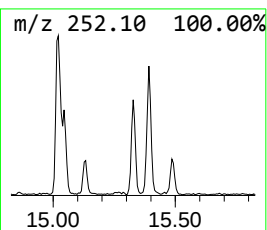
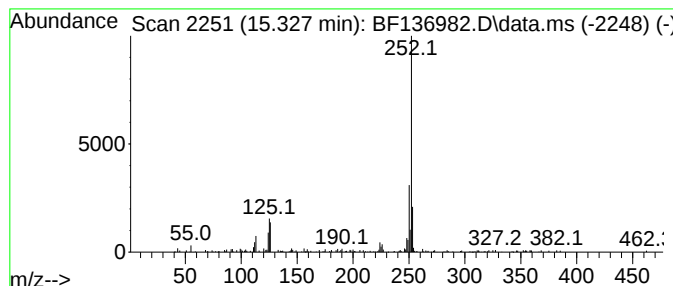
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	3.48 ng	81892	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Perylene	252	C20H12	000198-55-0	94
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136982.D
Acq On : 05 Jan 2024 18:29
Operator : CG\JU
Sample : 06015-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317-0-2

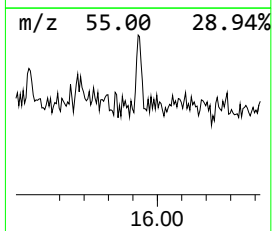
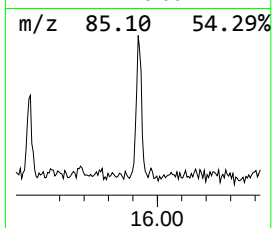
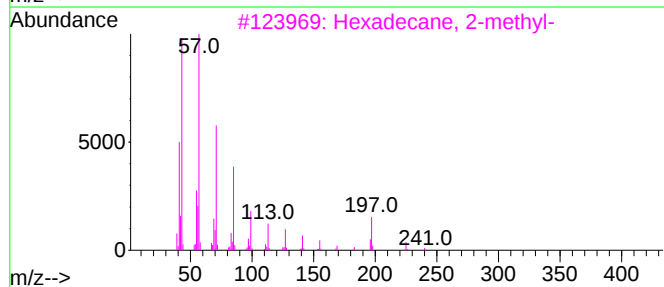
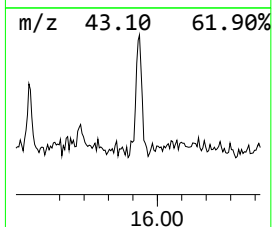
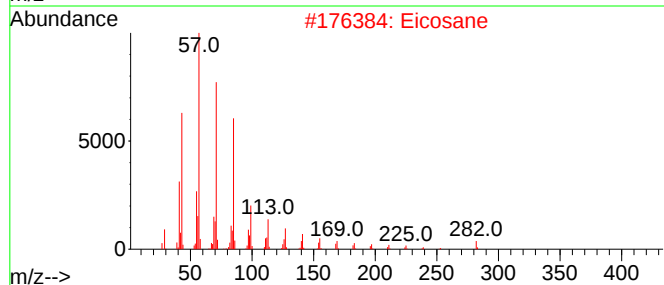
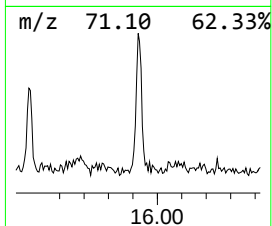
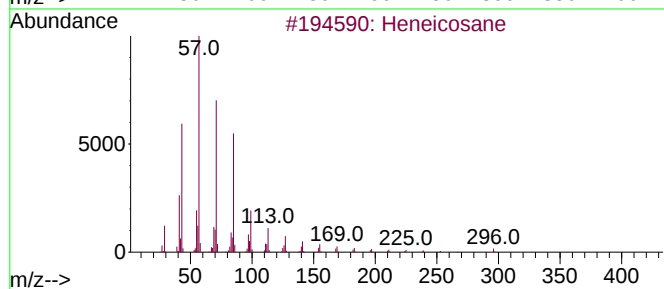
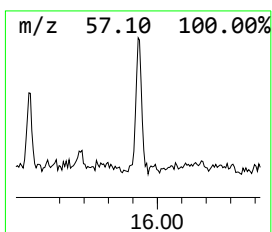
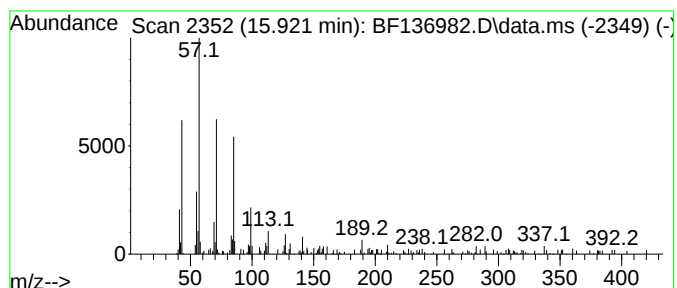
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	3.55 ng	83694	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Eicosane	282	C20H42	000112-95-8	81
3			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	78
4			Tetracosane	338	C24H50	000646-31-1	74
5			6,6-Diethylhooctadecane	310	C22H46	1000360-41-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136982.D
Acq On : 05 Jan 2024 18:29
Operator : CG\JU
Sample : 06015-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
2-Pentanone, 4-...	5.016	2.0	ng	35325	1	6.781	351354	20.0
n-Hexadecanoic ...	11.845	5.7	ng	118665	4	11.310	413531	20.0
4H-Cyclopenta[d...]	11.928	2.1	ng	42853	4	11.310	413531	20.0
Nonadecane	15.086	2.6	ng	61171	6	15.457	471093	20.0
Benzo[e]pyrene	15.327	3.5	ng	81892	6	15.457	471093	20.0
Heneicosane	15.921	3.5	ng	83694	6	15.457	471093	20.0