

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
 Data File : BF139780.D
 Acq On : 11 Oct 2024 17:42
 Operator : RC/JU
 Sample : P4353-01 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CF-400-COMP-43

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-BF100124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	6	21	rVB	954109	1328332	100.00%	14.320%
2	2.463	57	63	69	rVB	9040	18185	1.37%	0.196%
3	5.075	502	507	517	rVB	37525	53134	4.00%	0.573%
4	5.487	572	577	592	rVB	549082	732359	55.13%	7.895%
5	6.498	744	749	778	rBV	490721	699095	52.63%	7.537%
6	6.869	807	812	817	rBV	330563	402939	30.33%	4.344%
7	7.428	902	907	916	rBV	328478	411473	30.98%	4.436%
8	7.686	946	951	962	rVB	9726	16281	1.23%	0.176%
9	8.151	1024	1030	1045	rVB	353458	453400	34.13%	4.888%
10	9.222	1207	1212	1222	rBV	586941	713660	53.73%	7.694%
11	9.763	1300	1304	1310	rBV	30648	38852	2.92%	0.419%
12	9.904	1323	1328	1338	rBV	374013	460080	34.64%	4.960%
13	10.316	1392	1398	1402	rBV2	9894	16632	1.25%	0.179%
14	10.616	1443	1449	1457	rBV	57943	75712	5.70%	0.816%
15	10.692	1457	1462	1473	rVV	323350	417075	31.40%	4.496%
16	11.392	1576	1581	1590	rBV	414283	547788	41.24%	5.906%
17	11.916	1662	1670	1677	rBV3	118299	221891	16.70%	2.392%
18	12.004	1681	1685	1688	rBV2	23098	33521	2.52%	0.361%
19	12.186	1711	1716	1719	rBV4	11798	19665	1.48%	0.212%
20	12.216	1719	1721	1727	rVB4	10813	14317	1.08%	0.154%
21	12.445	1755	1760	1762	rBV	38253	56410	4.25%	0.608%
22	12.474	1762	1765	1771	rVV4	24600	48562	3.66%	0.524%
23	12.533	1771	1775	1782	rVB4	18658	32045	2.41%	0.345%
24	12.604	1783	1787	1791	rBV	69349	88123	6.63%	0.950%
25	12.651	1791	1795	1797	rBV2	10059	15360	1.16%	0.166%
26	12.698	1800	1803	1807	rBV	27300	36472	2.75%	0.393%
27	12.833	1821	1826	1832	rBV	102122	152698	11.50%	1.646%
28	12.892	1833	1836	1839	rVB2	18636	21835	1.64%	0.235%
29	12.974	1845	1850	1858	rVB	677967	877624	66.07%	9.461%
30	13.051	1859	1863	1870	rBV3	29284	60697	4.57%	0.654%
31	13.157	1875	1881	1885	rVB3	33717	69652	5.24%	0.751%
32	13.268	1897	1900	1905	rVB	30130	34273	2.58%	0.369%
33	13.363	1912	1916	1918	rBV	30486	39447	2.97%	0.425%
34	13.392	1918	1921	1924	rVB	22391	26868	2.02%	0.290%
35	13.886	2001	2005	2013	rVB4	32940	67979	5.12%	0.733%
36	14.033	2025	2030	2041	rVB2	355374	549101	41.34%	5.920%

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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-BF100124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.786	2155	2158	2164	rVB2	63629	92596	6.97%	0.998%
38	15.509	2276	2281	2293	rVB	198485	331748	24.97%	3.576%

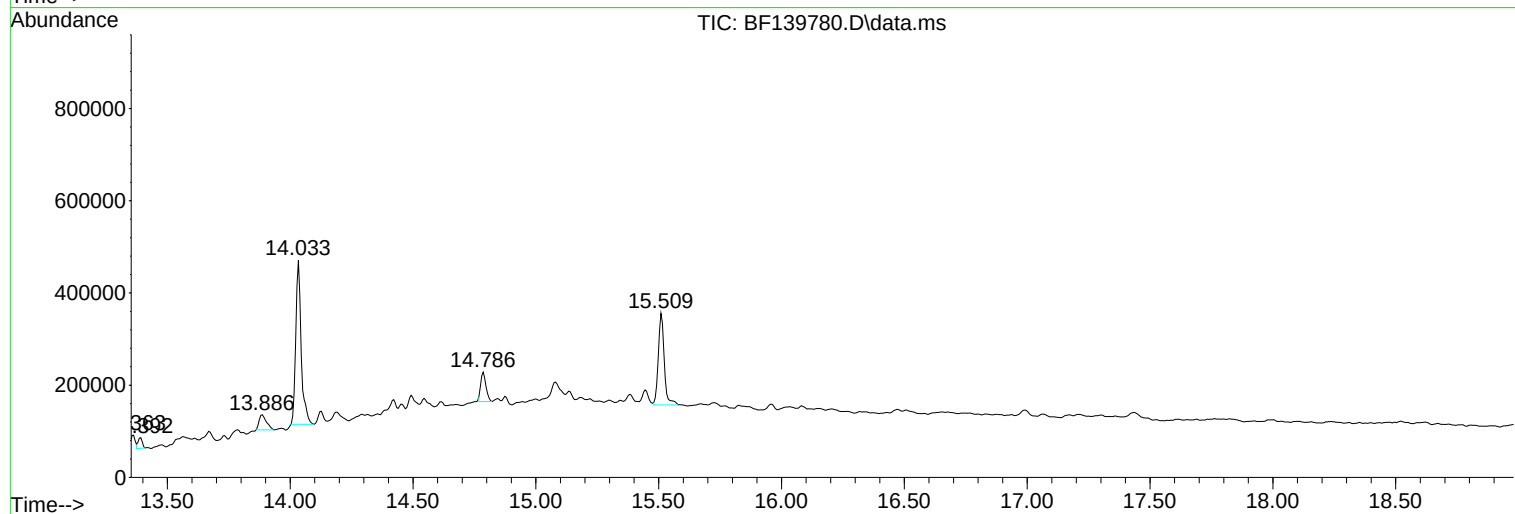
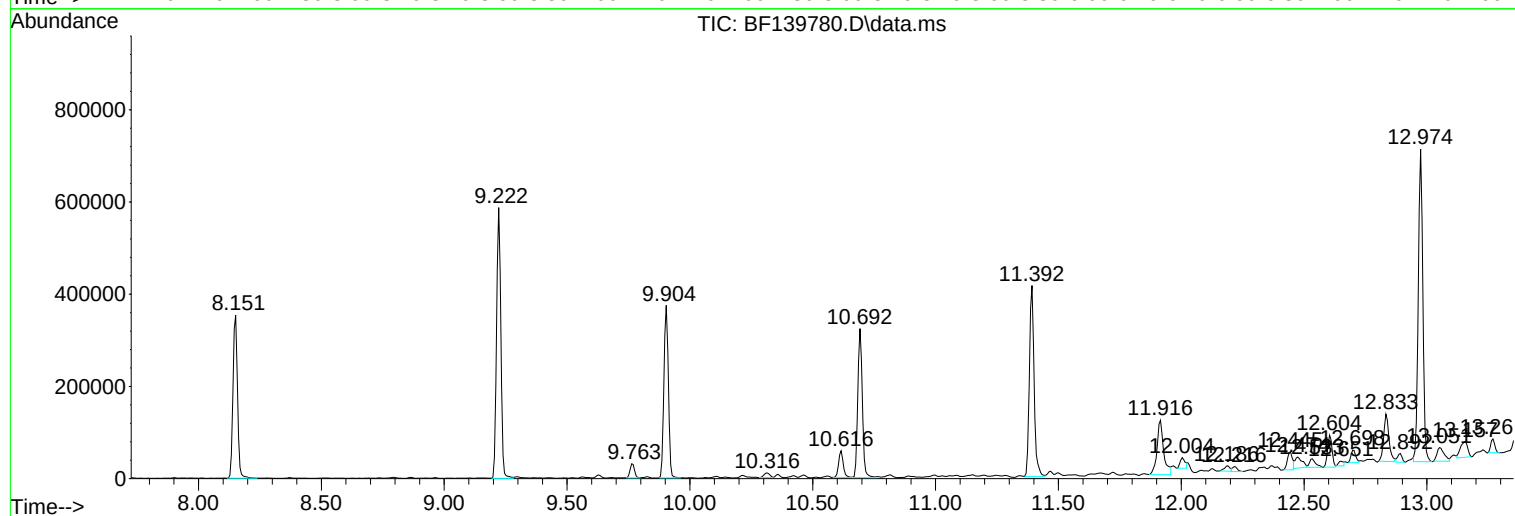
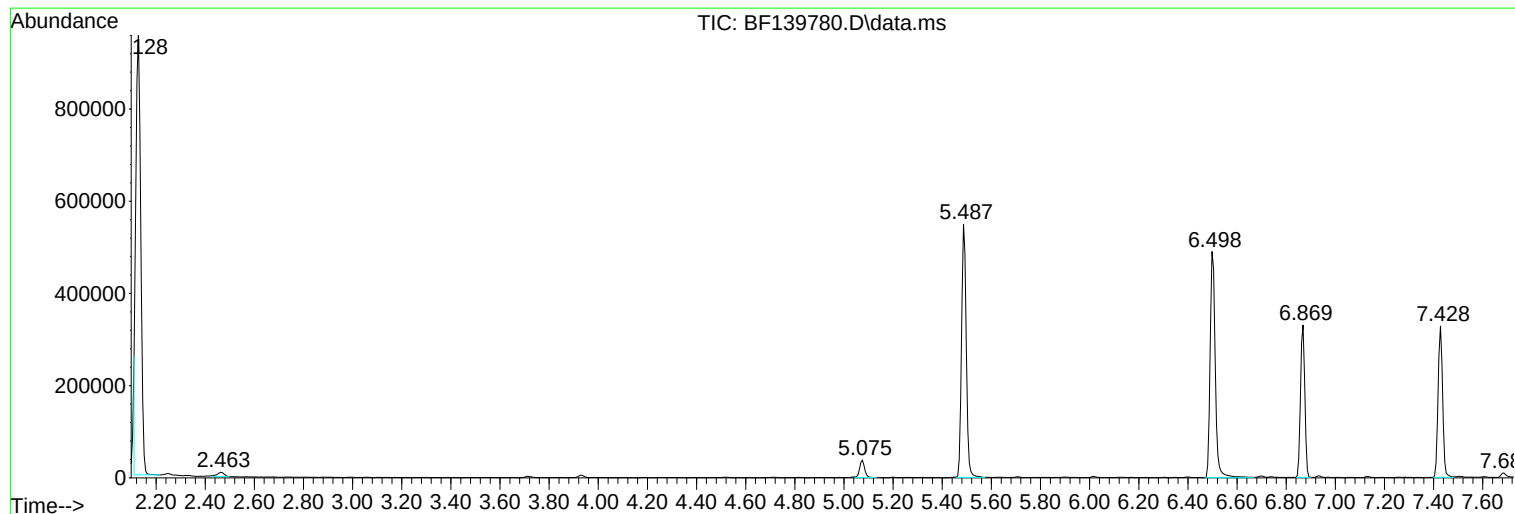
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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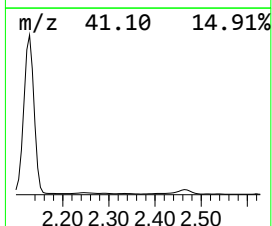
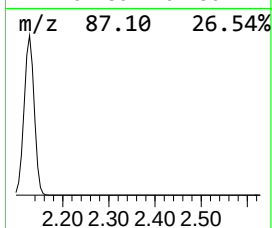
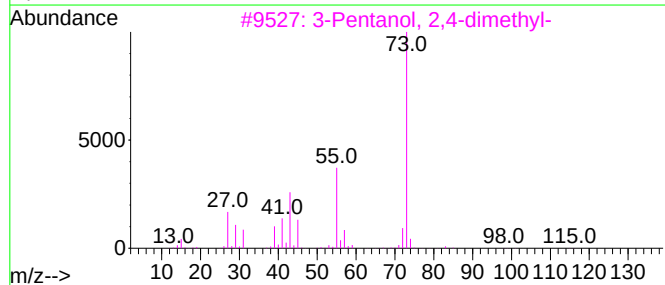
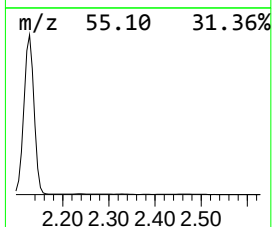
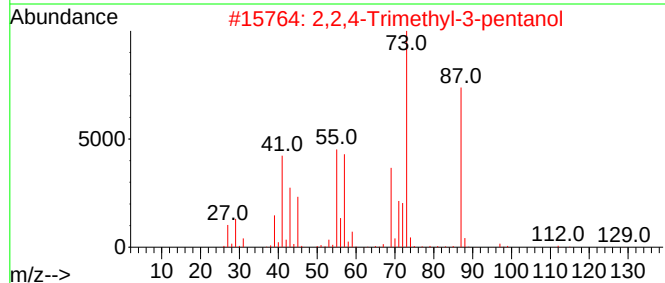
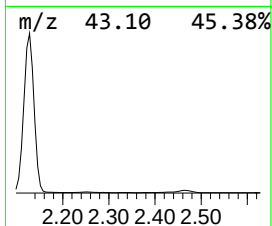
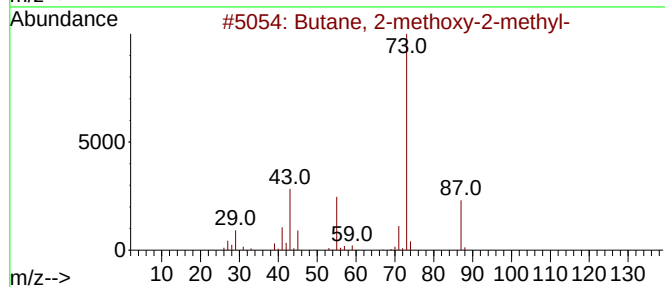
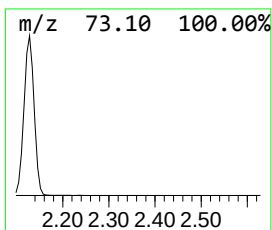
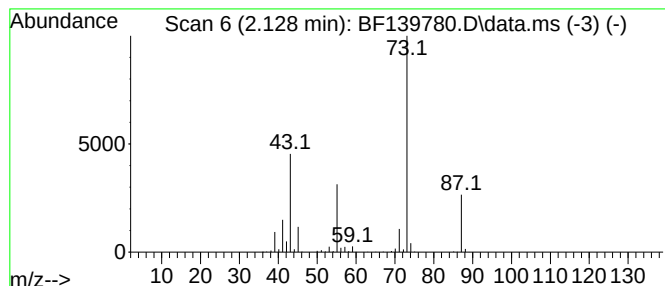
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.128	65.93 ng	1328330	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	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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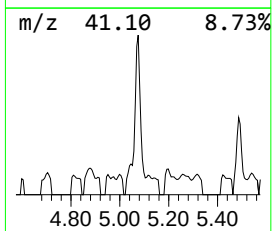
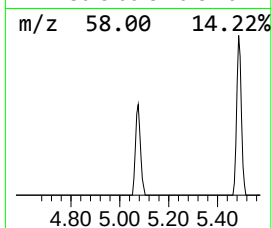
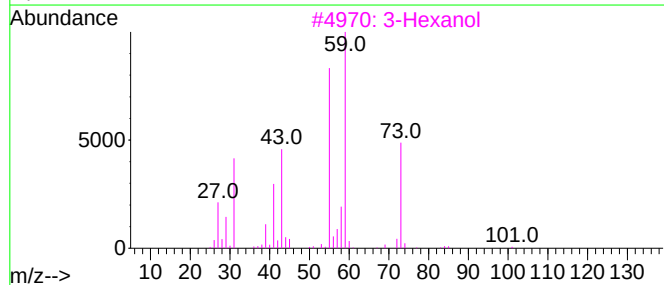
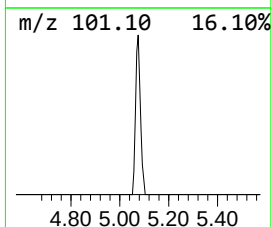
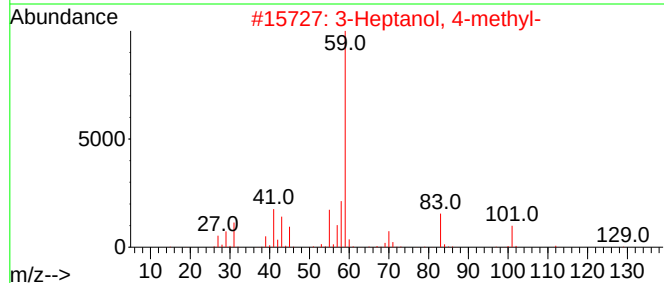
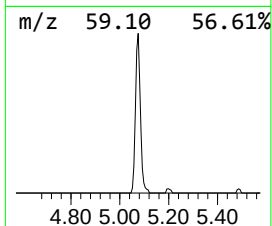
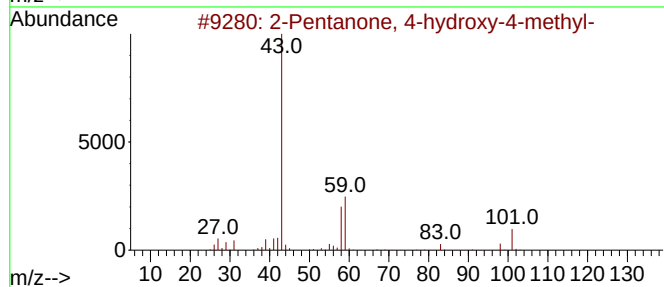
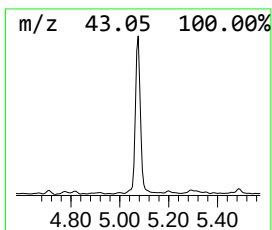
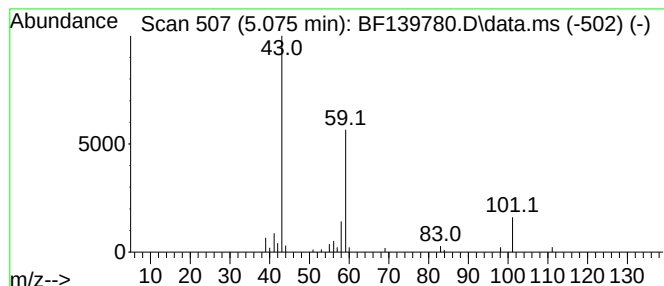
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.075	2.64 ng	53134	1,4-Dichlorobenzene-d4	6.869	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28



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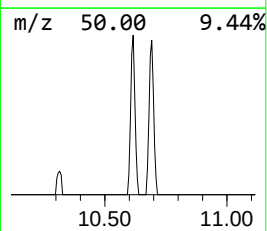
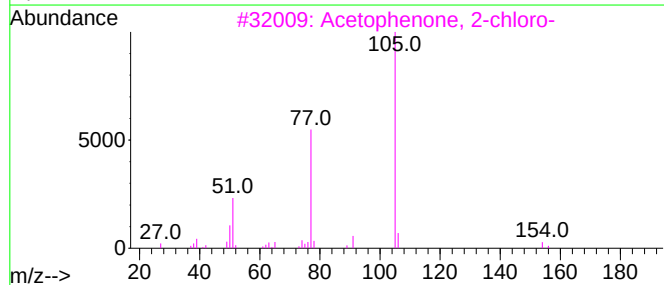
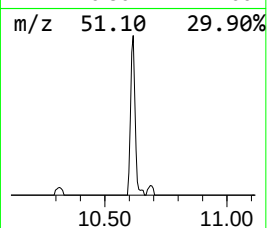
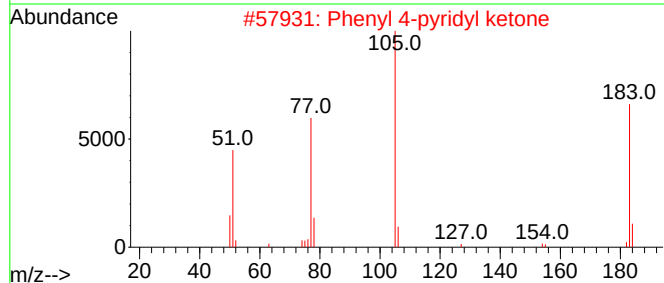
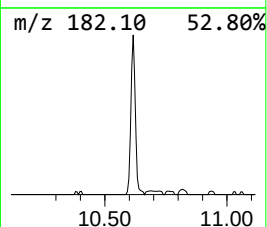
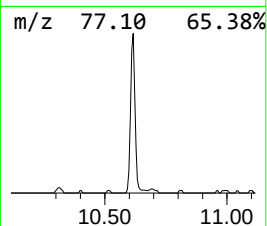
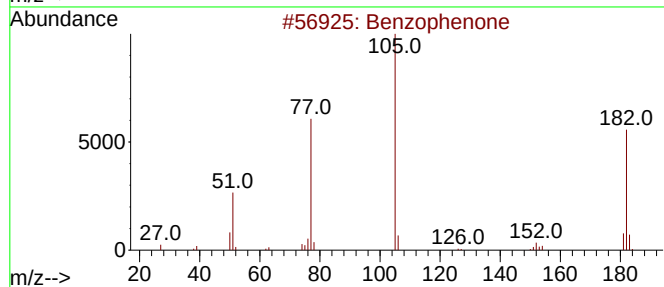
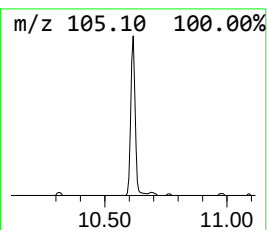
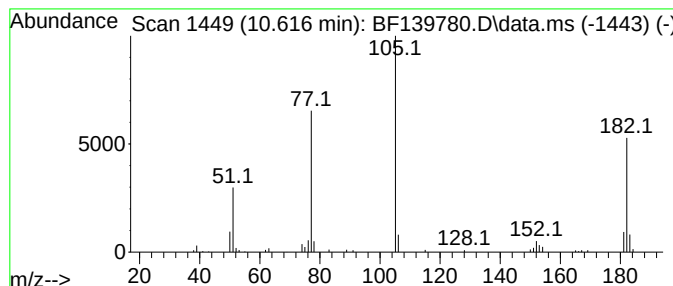
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	3.29 ng	75712	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	53
4			Benzoylformic acid	150	C8H6O3	000611-73-4	49
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47



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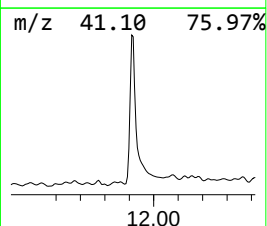
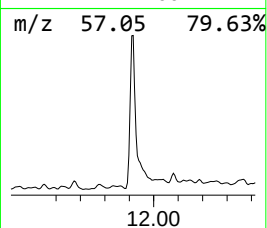
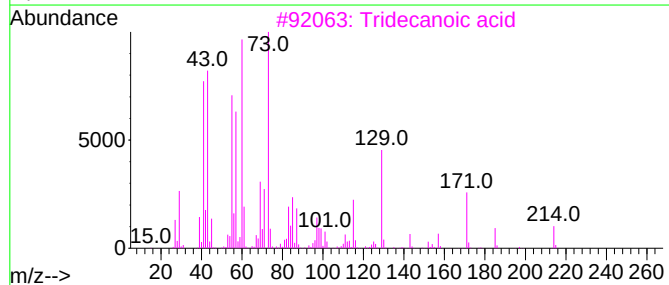
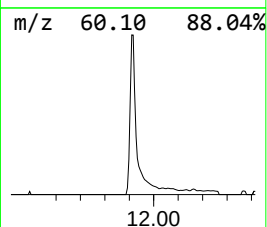
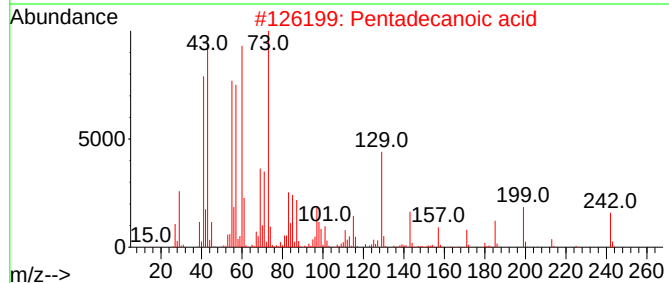
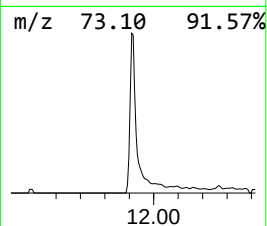
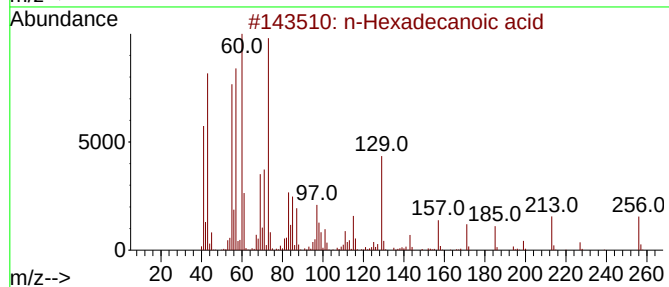
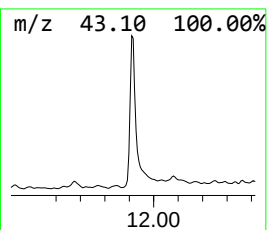
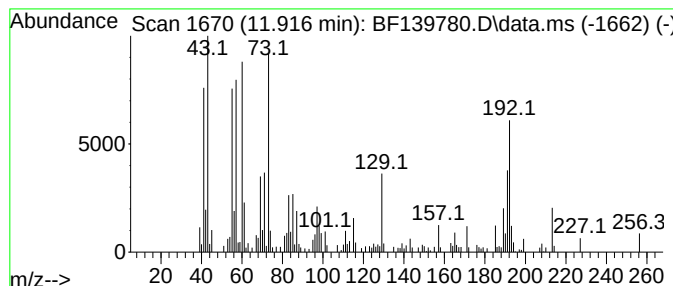
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	8.10 ng	221891	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	78
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	59



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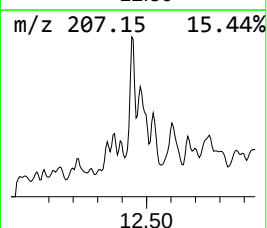
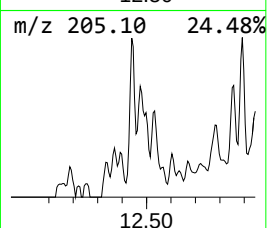
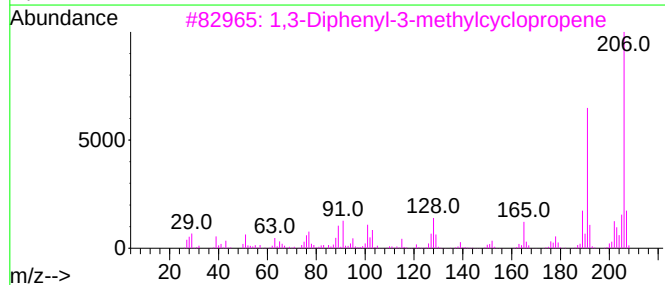
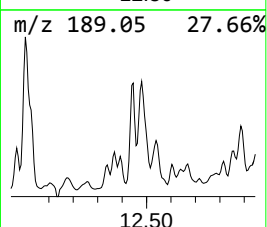
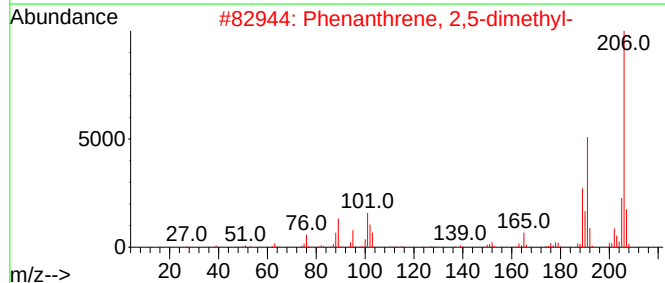
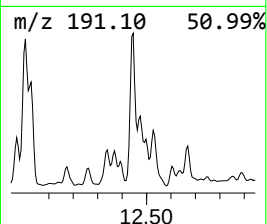
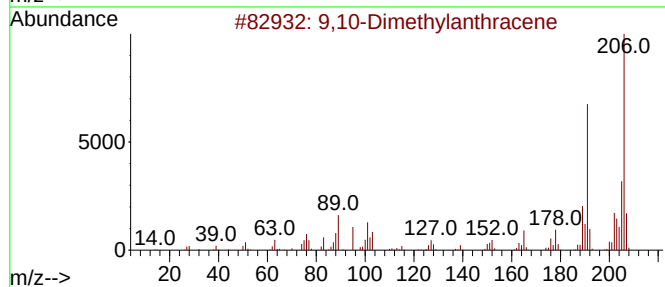
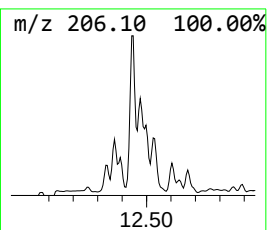
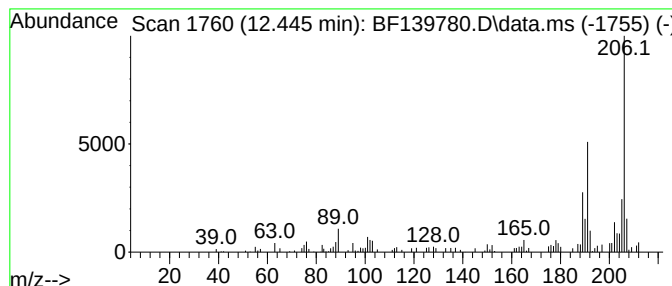
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9,10-Dimethylantracene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	2.06 ng	56410	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,10-Dimethylantracene	206	C16H14	000781-43-1	95
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
3			1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	90
4			1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	90
5			di-p-Tolylacetylene	206	C16H14	002789-88-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139780.D
Acq On : 11 Oct 2024 17:42
Operator : RC/JU
Sample : P4353-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

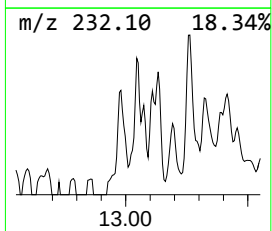
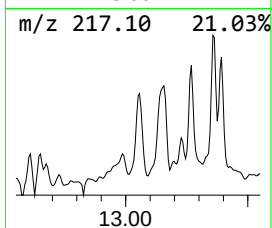
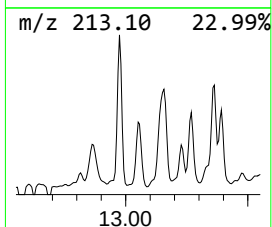
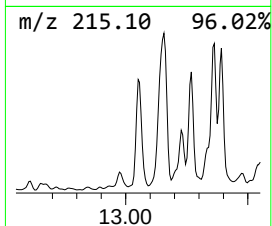
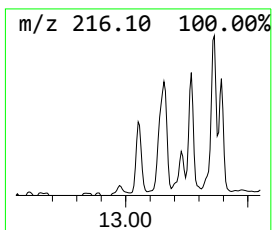
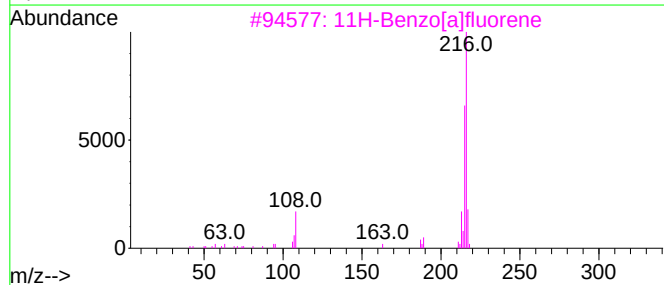
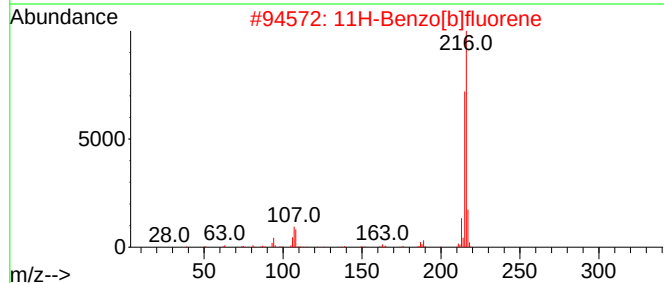
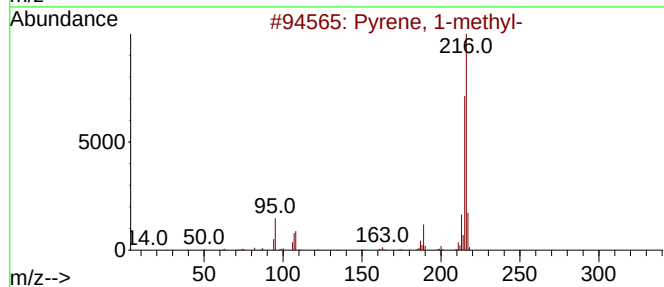
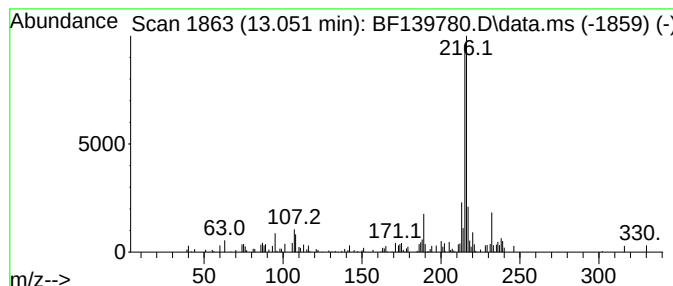
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ClientSampleId :
CF-400-COMP-43

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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 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.051	2.21 ng	60697	Chrysene-d12		14.033	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-		216	C17H12	002381-21-7	91
2	11H-Benzo[b]fluorene		216	C17H12	000243-17-4	83
3	11H-Benzo[a]fluorene		216	C17H12	000238-84-6	76
4	Fluoranthene, 2-methyl-		216	C17H12	033543-31-6	76
5	Pyrene, 2-methyl-		216	C17H12	003442-78-2	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139780.D
Acq On : 11 Oct 2024 17:42
Operator : RC/JU
Sample : P4353-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-400-COMP-43

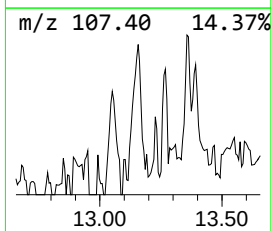
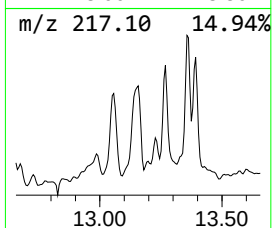
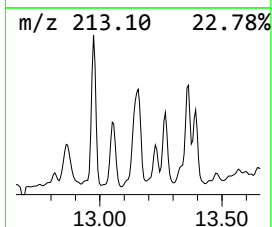
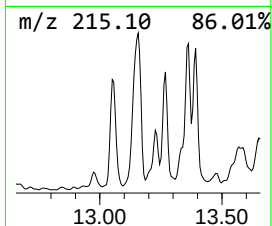
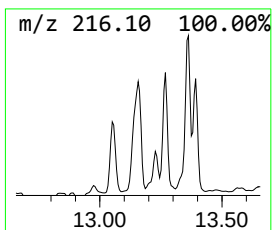
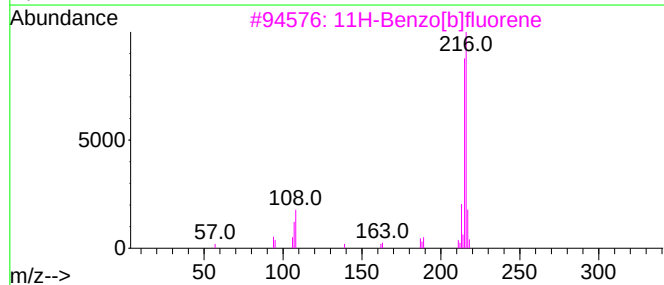
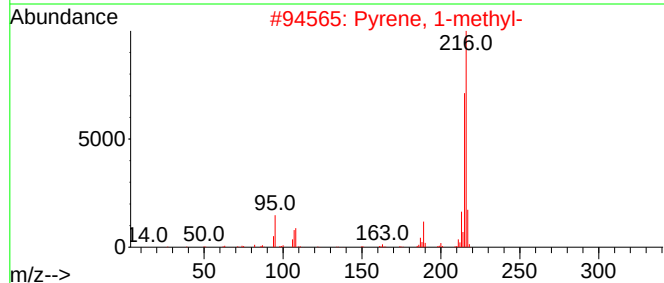
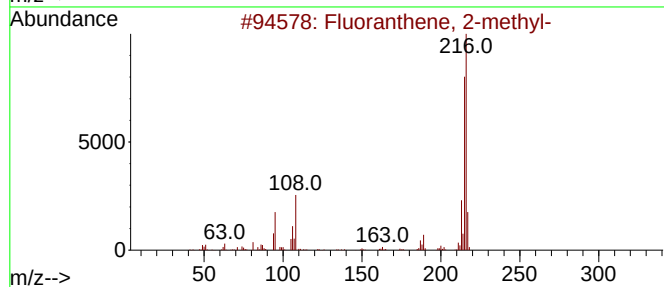
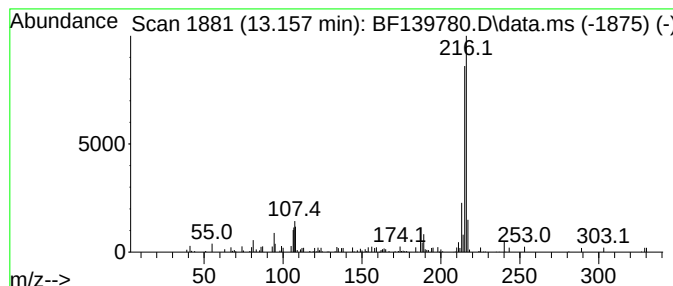
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Fluoranthene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	2.54 ng	69652	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	81
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	81
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	76
5			Pyrene, 2-methyl-	216	C17H12	003442-78-2	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139780.D
Acq On : 11 Oct 2024 17:42
Operator : RC/JU
Sample : P4353-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-400-COMP-43

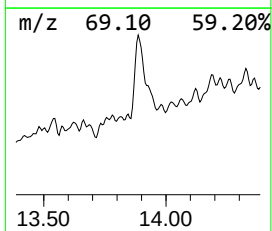
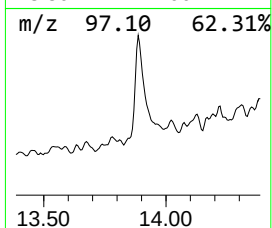
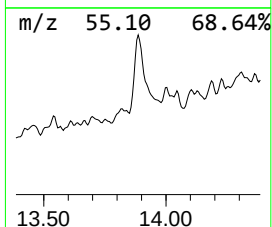
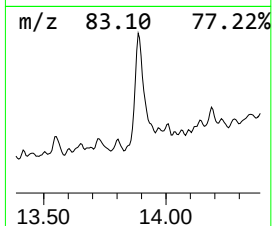
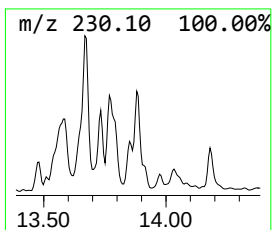
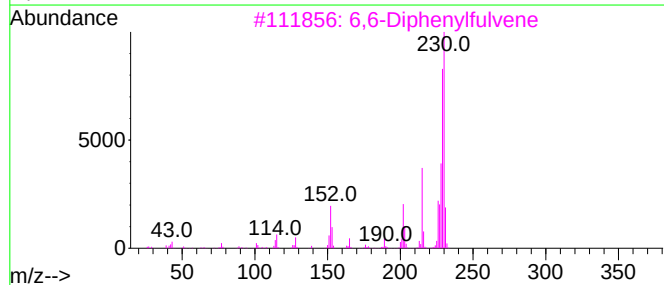
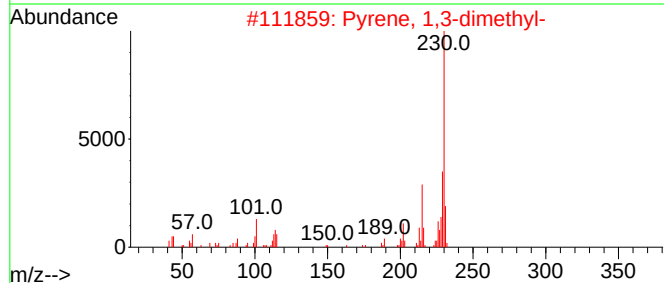
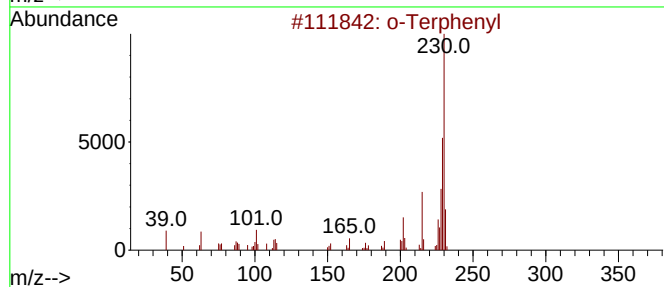
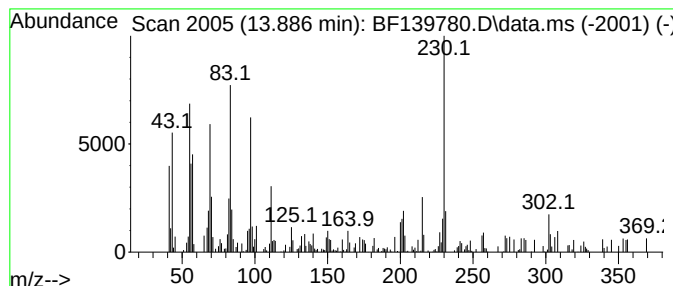
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.886 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.48 ng	67979	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Terphenyl	230	C18H14	000084-15-1	46
2			Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	35
3			6,6-Diphenylfulvene	230	C18H14	002175-90-8	30
4			2,5-Methano-2H-thieno[3,2-b]thio...	230	C10H14O2S2	035636-01-2	25
5			Benzonitrile, 4-(2-cyano-2-pheny...	230	C16H10N2	061469-58-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139780.D
Acq On : 11 Oct 2024 17:42
Operator : RC/JU
Sample : P4353-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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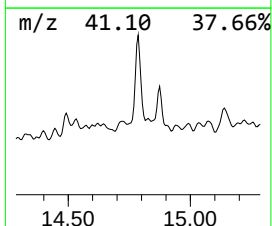
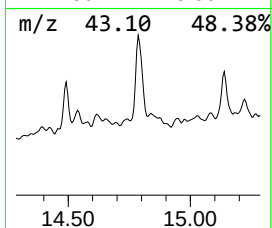
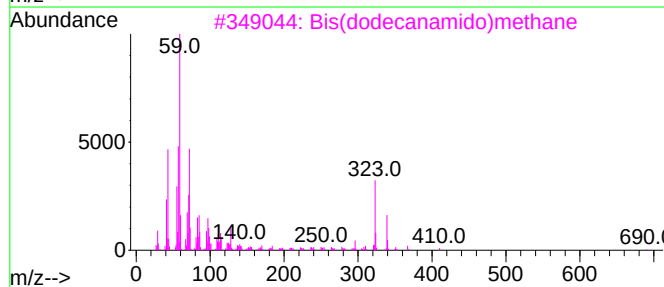
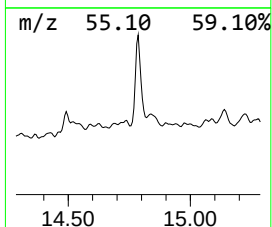
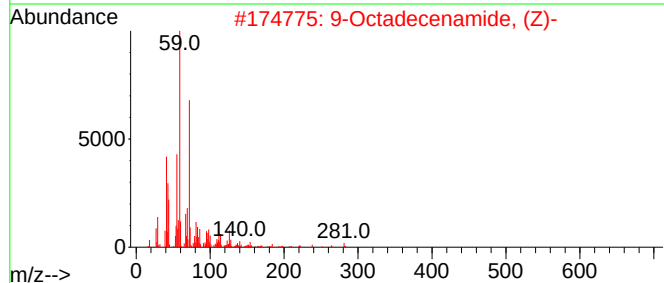
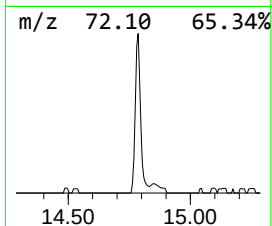
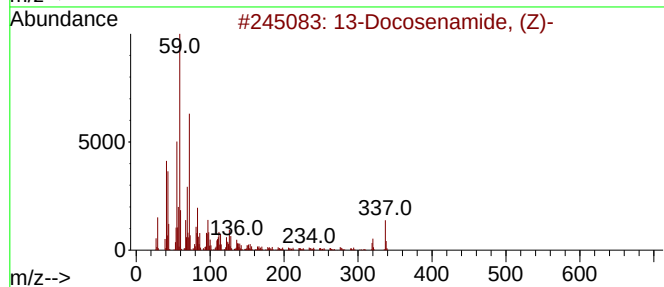
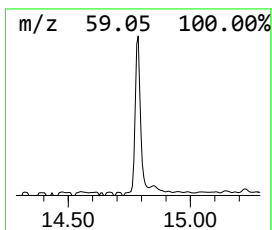
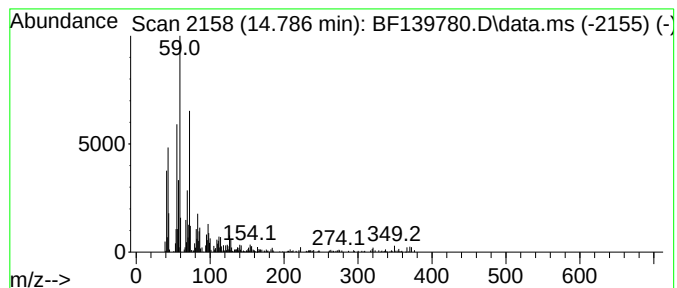
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	5.58 ng	92596	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3			Bis(dodecanamido)methane	691	C45H90N2O2	010436-15-4	72
4			7-Nonenamide	155	C9H17NO	090949-53-4	64
5			Palmitoleamide	253	C16H31NO	106010-22-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101124\
Data File : BF139780.D
Acq On : 11 Oct 2024 17:42
Operator : RC/JU
Sample : P4353-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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
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2-Pentanone, 4-...	5.075	2.6	ng	53134	1	6.869	402939	20.0
Benzophenone	10.616	3.3	ng	75712	3	9.904	460080	20.0
n-Hexadecanoic ...	11.916	8.1	ng	221891	4	11.392	547788	20.0
9,10-Dimethylan...	12.445	2.1	ng	56410	4	11.392	547788	20.0
Pyrene, 1-methyl-	13.051	2.2	ng	60697	5	14.033	549101	20.0
Fluoranthene, 2...	13.157	2.5	ng	69652	5	14.033	549101	20.0
unknown13.886	13.886	2.5	ng	67979	5	14.033	549101	20.0
13-Docosenamide...	14.786	5.6	ng	92596	6	15.509	331748	20.0