

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
 Data File : BF139400.D
 Acq On : 17 Sep 2024 14:17
 Operator : RC/JU
 Sample : P3985-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-7

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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139400.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	9	17	24	rVB	644518	980338	57.26%	8.005%
2	3.399	216	222	248	rBV	27738	67691	3.95%	0.553%
3	5.099	501	511	518	rVB	74979	109773	6.41%	0.896%
4	5.499	573	579	584	rBV	1062064	1398530	81.68%	11.419%
5	6.504	744	750	755	rBV	1129927	1532946	89.54%	12.517%
6	6.698	779	783	790	rBV	21400	28294	1.65%	0.231%
7	6.875	808	813	818	rVB	347142	421112	24.60%	3.438%
8	7.440	902	909	914	rBV	699881	939646	54.88%	7.672%
9	7.693	947	952	958	rVB	25302	32070	1.87%	0.262%
10	8.157	1026	1031	1036	rBV	430826	527111	30.79%	4.304%
11	8.469	1079	1084	1095	rVB	44713	58738	3.43%	0.480%
12	9.234	1208	1214	1219	rBV	1377142	1712117	100.00%	13.980%
13	9.910	1324	1329	1334	rBV	470285	575787	33.63%	4.701%
14	10.004	1340	1345	1350	rBV	27377	39983	2.34%	0.326%
15	10.622	1445	1450	1455	rBV	131098	159264	9.30%	1.300%
16	10.698	1457	1463	1475	rVV	792789	996667	58.21%	8.138%
17	10.928	1493	1502	1509	rBV	16717	21391	1.25%	0.175%
18	11.392	1576	1581	1590	rBV	405904	529379	30.92%	4.322%
19	11.551	1601	1608	1614	rBV	12057	17993	1.05%	0.147%
20	11.916	1662	1670	1682	rBV3	64629	100954	5.90%	0.824%
21	12.604	1783	1787	1792	rBV	26556	31718	1.85%	0.259%
22	12.698	1798	1803	1810	rBV3	12713	20816	1.22%	0.170%
23	12.833	1817	1826	1831	rBV	23872	37066	2.16%	0.303%
24	12.980	1845	1851	1856	rBV	826575	1073142	62.68%	8.762%
25	13.874	1998	2003	2013	rBV	43260	71599	4.18%	0.585%
26	14.027	2024	2029	2043	rVB	264395	358578	20.94%	2.928%
27	14.504	2105	2110	2123	rBV4	15087	35567	2.08%	0.290%
28	15.069	2201	2206	2214	rBV	13168	28112	1.64%	0.230%
29	15.145	2215	2219	2222	rBV	13162	18476	1.08%	0.151%
30	15.498	2273	2279	2292	rBV	178556	281004	16.41%	2.294%
31	17.145	2553	2559	2567	rVB5	19603	41340	2.41%	0.338%

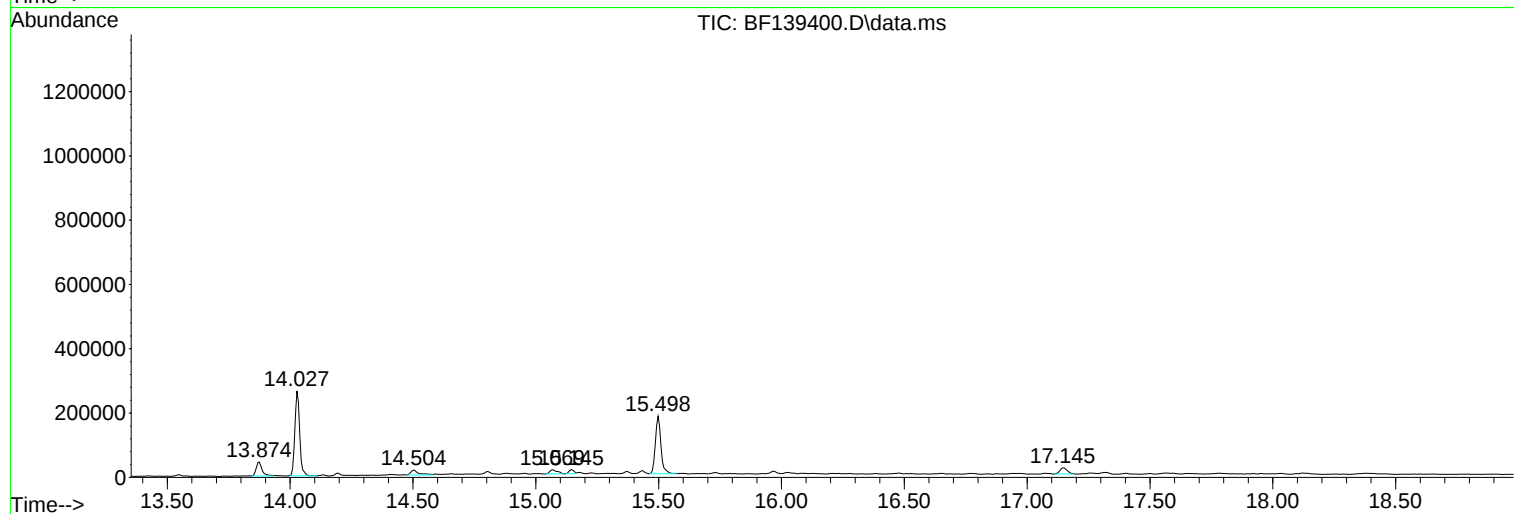
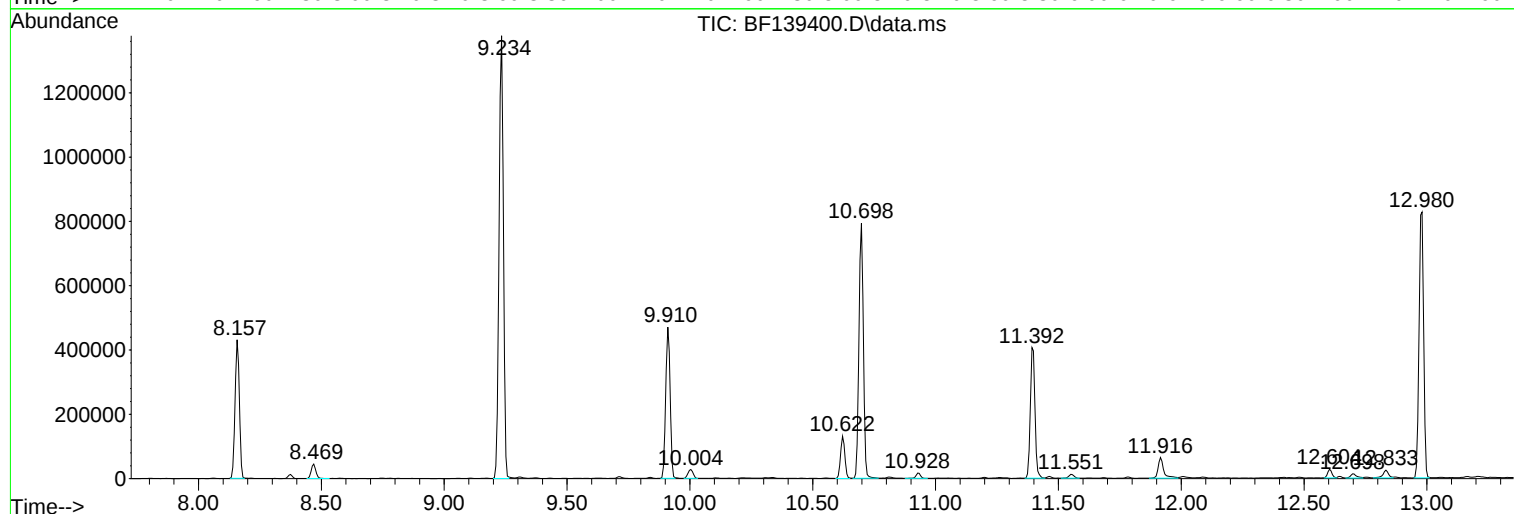
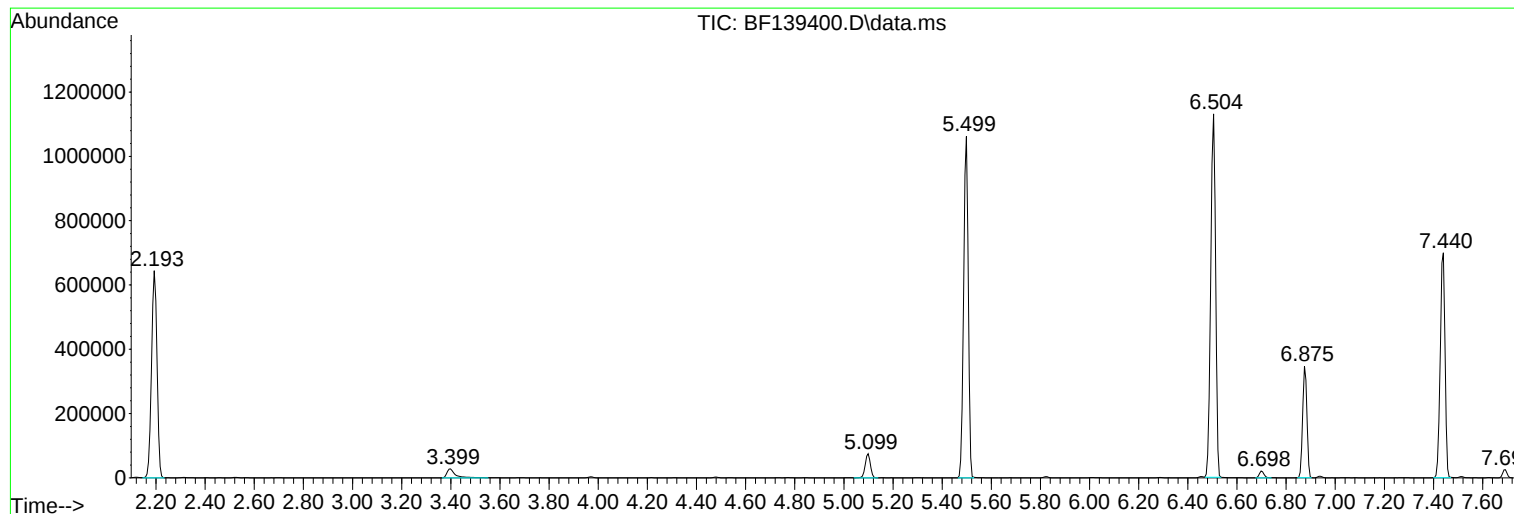
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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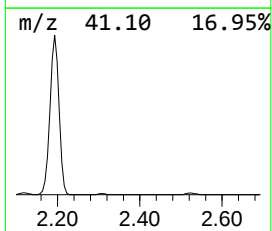
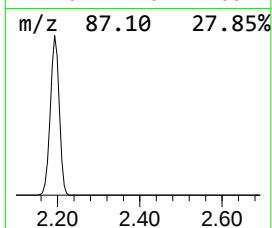
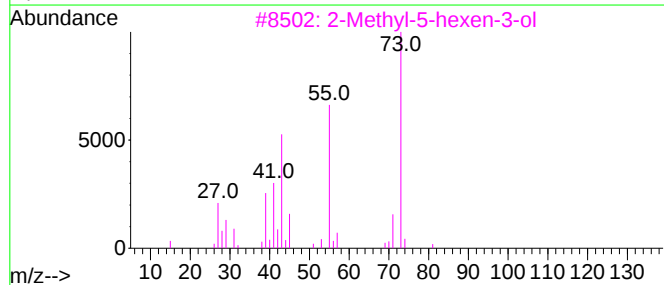
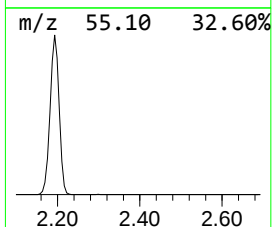
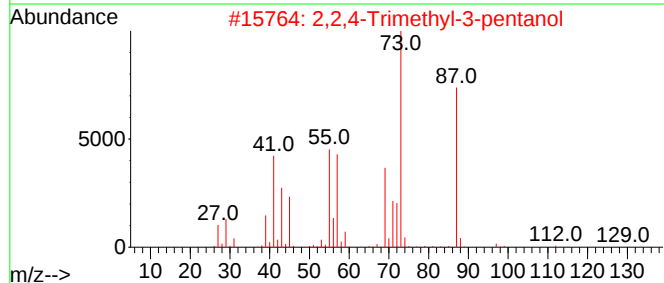
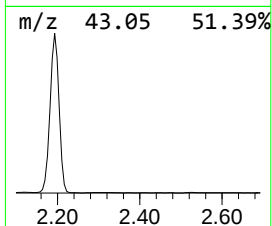
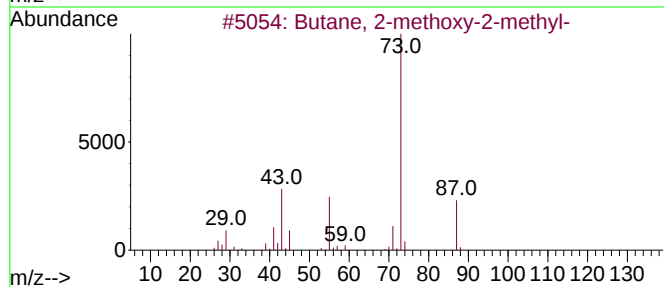
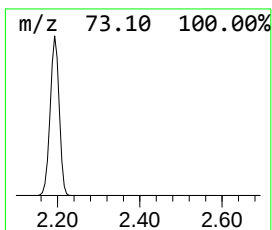
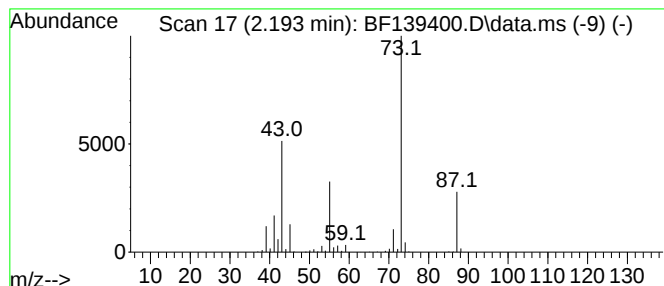
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	46.56 ng	980338	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	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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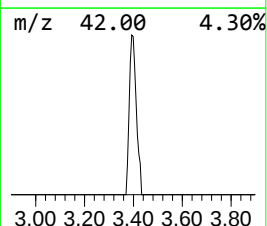
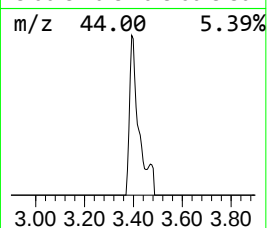
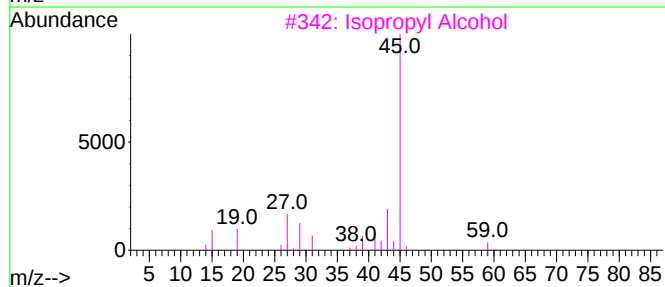
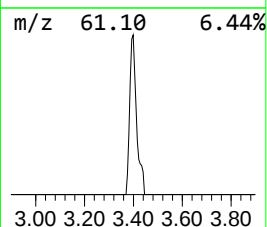
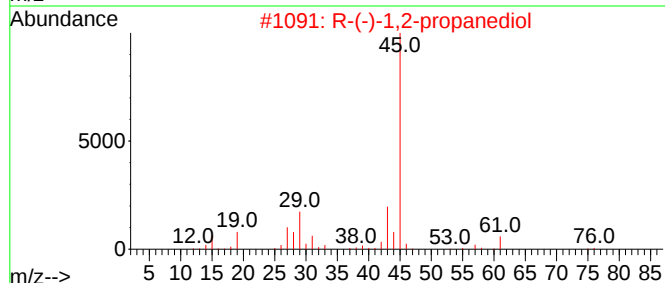
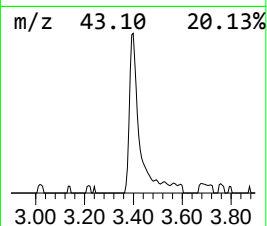
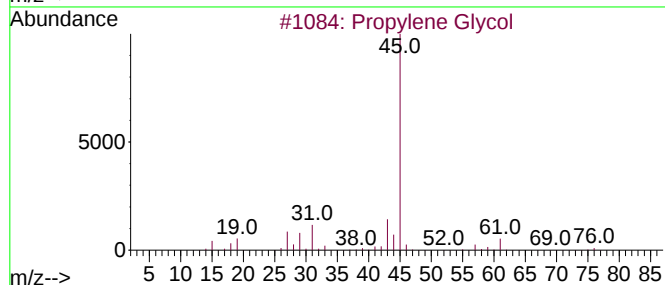
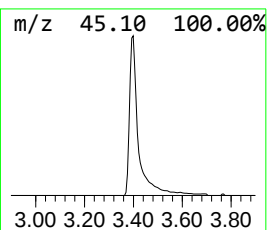
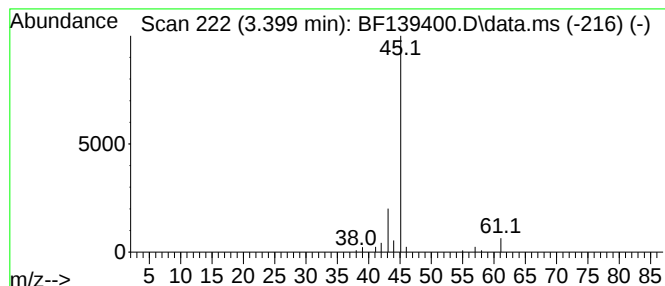
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Peak Number 2 unknown3.399 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	3.21 ng	67691	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	9
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5			Formamide	45	CH3NO	000075-12-7	5



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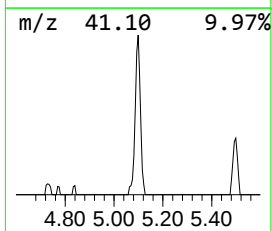
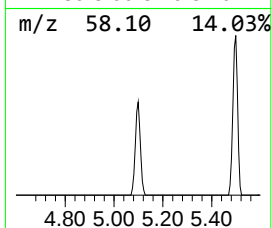
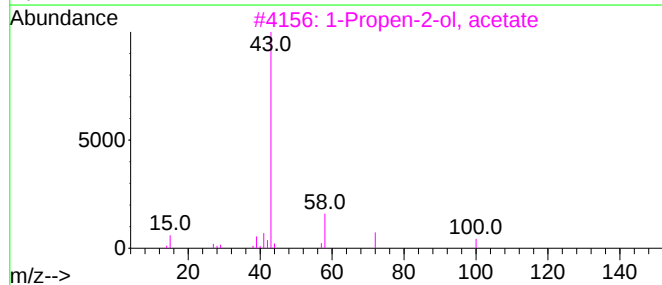
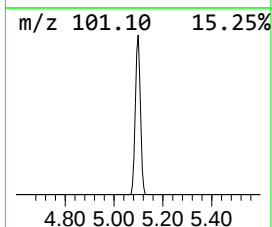
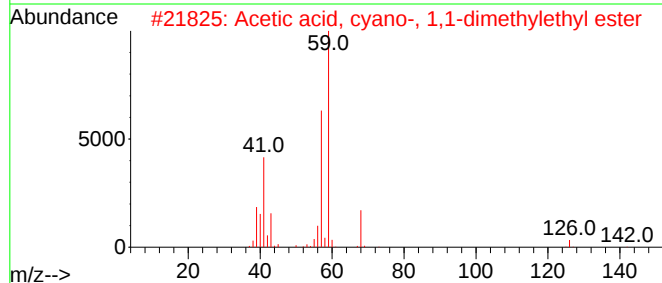
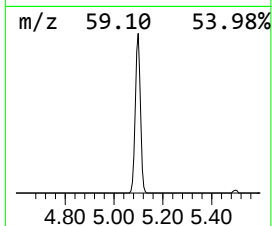
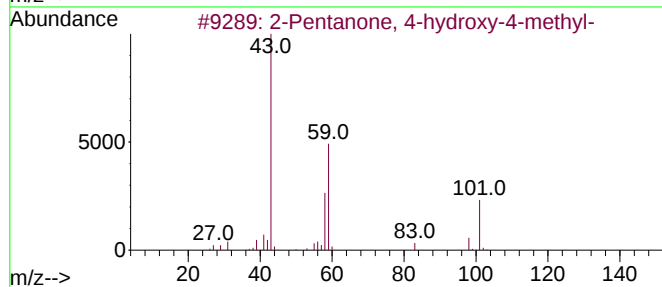
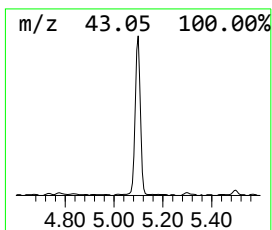
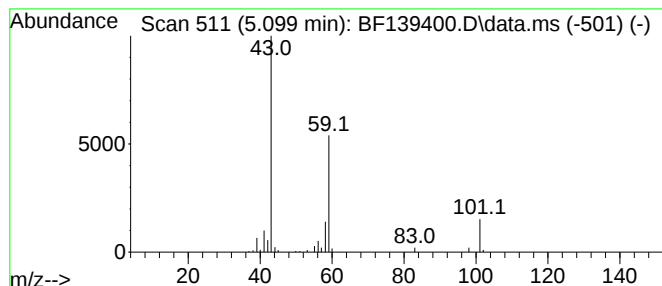
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	5.21 ng	109773	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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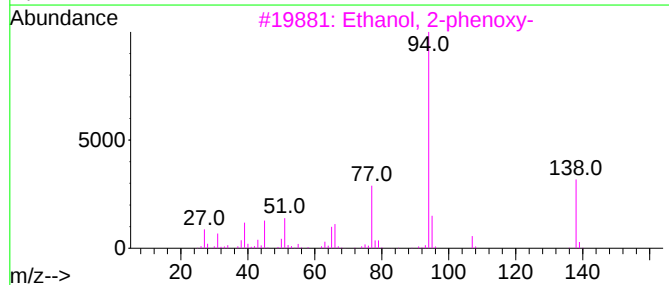
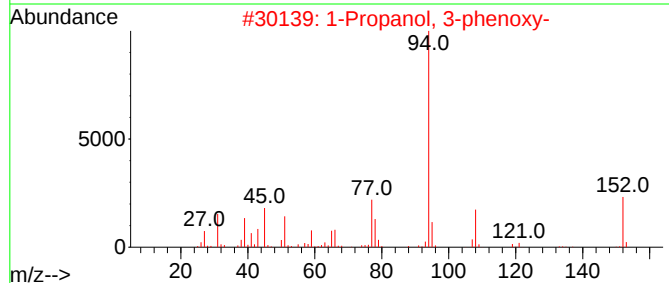
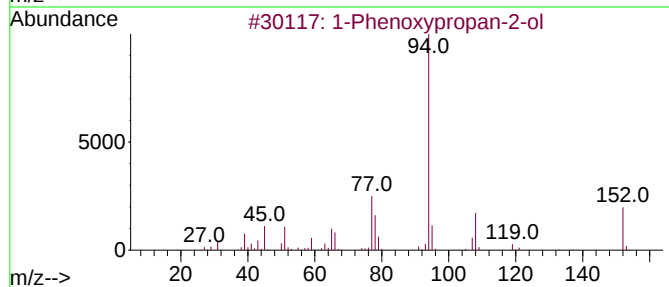
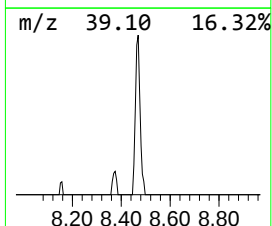
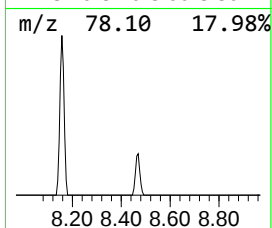
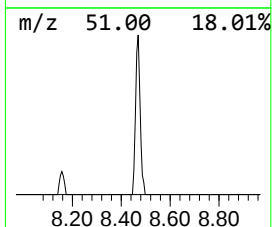
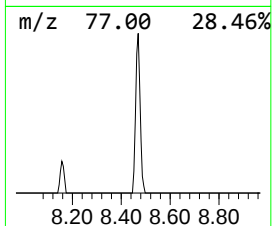
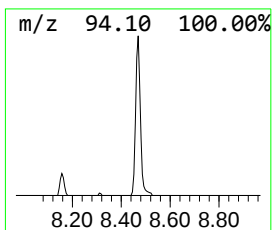
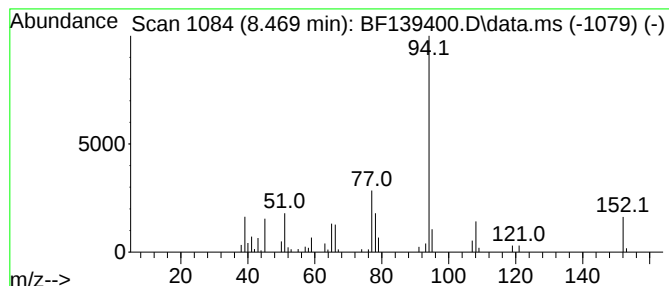
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	2.23 ng	58738	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	80
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53
5			2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53



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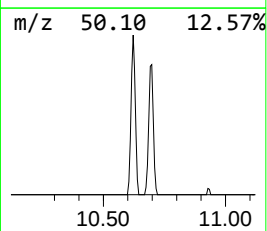
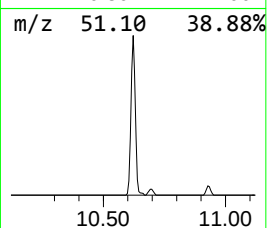
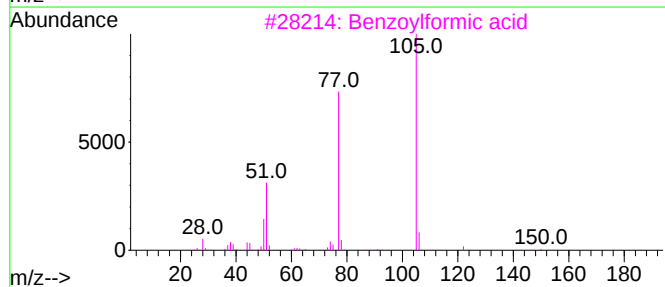
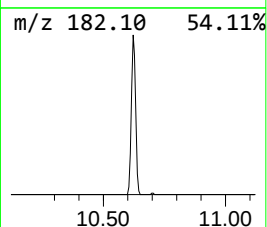
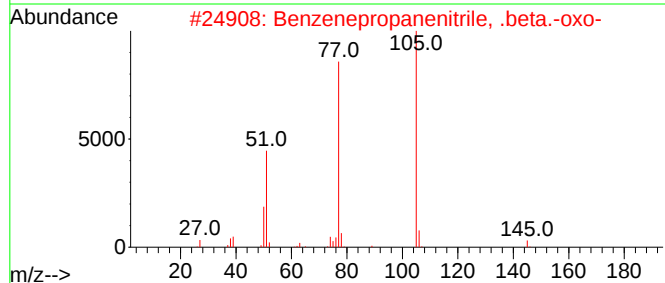
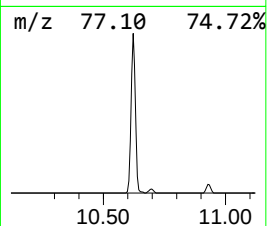
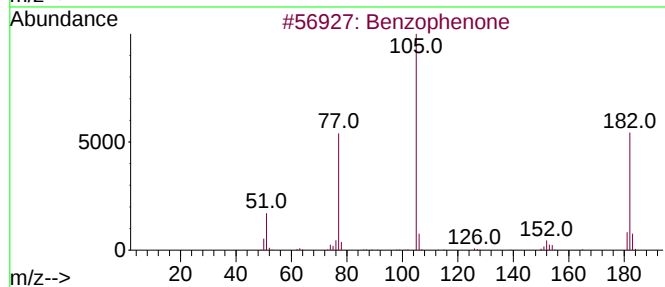
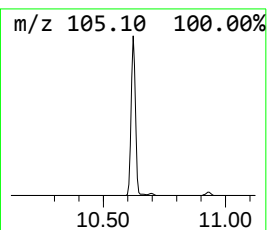
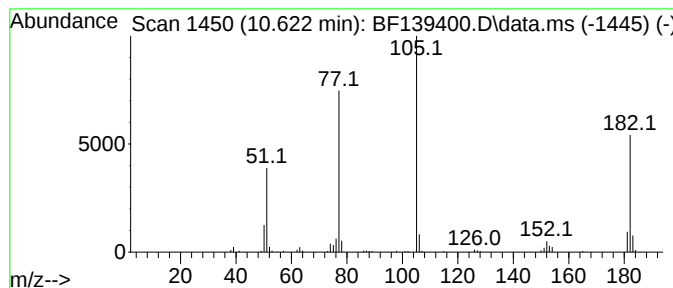
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	5.53 ng	159264	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	58
3			Benzoylformic acid	150	C8H6O3	000611-73-4	58
4			2-Bromoisobutyrophenone	226	C10H11BrO	010409-54-8	53
5			Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	53



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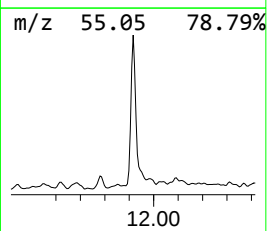
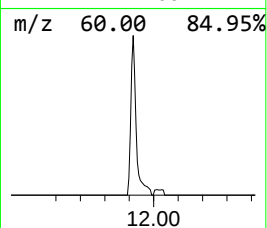
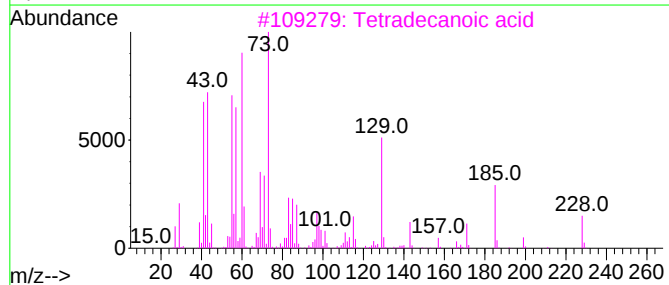
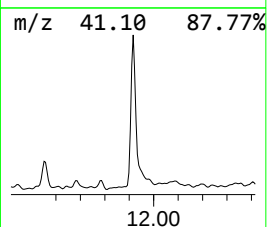
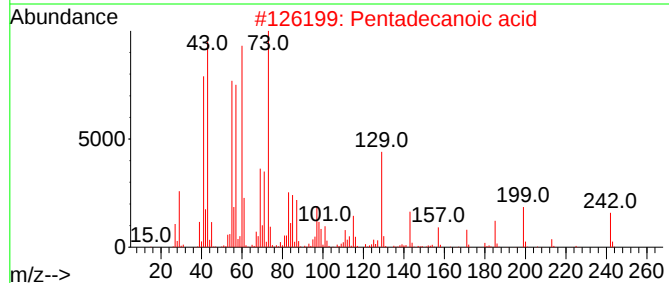
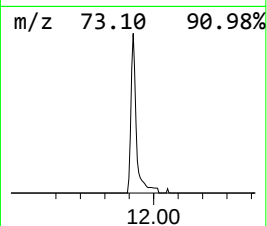
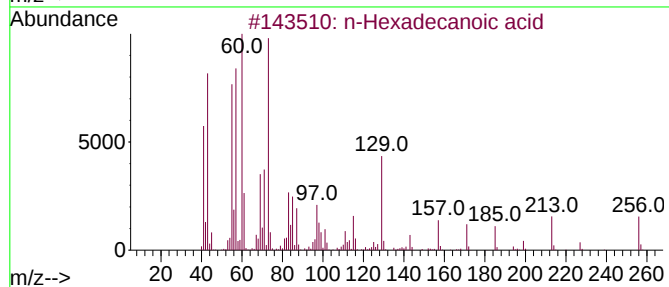
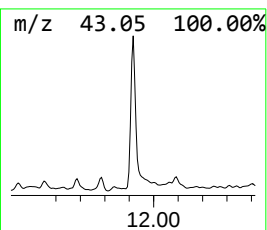
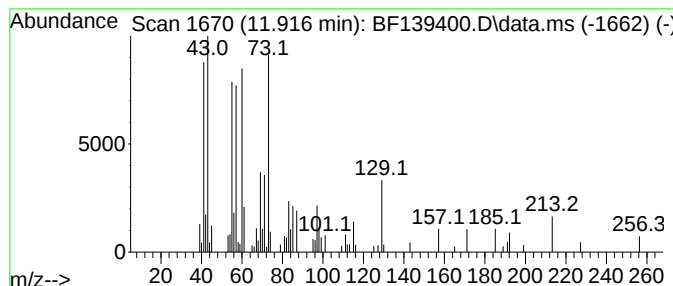
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.81 ng	100954	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
Data File : BF139400.D
Acq On : 17 Sep 2024 14:17
Operator : RC/JU
Sample : P3985-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

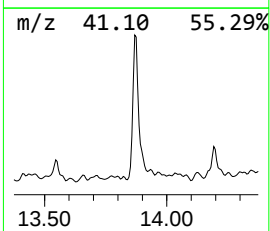
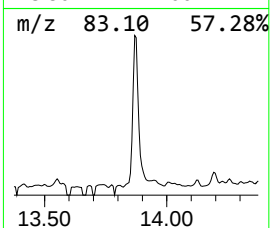
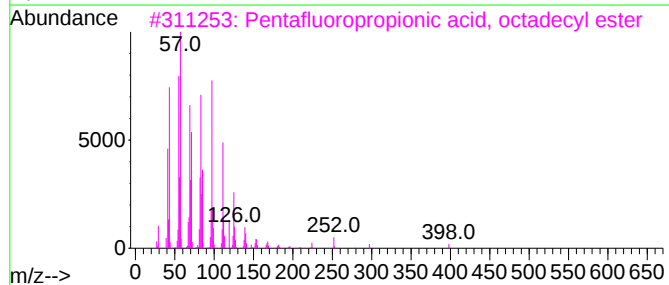
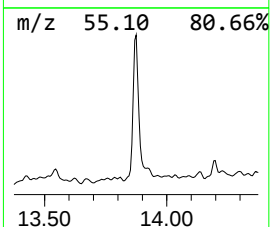
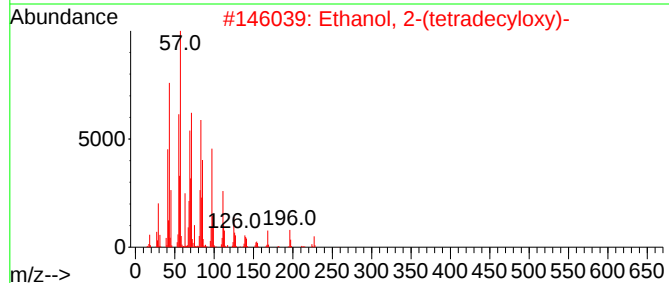
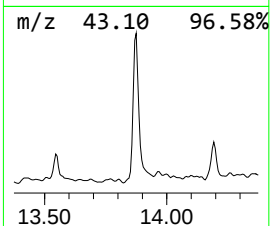
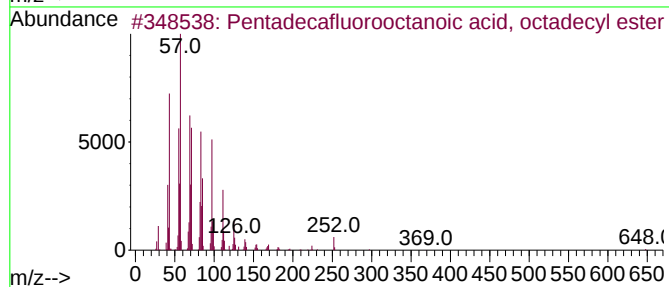
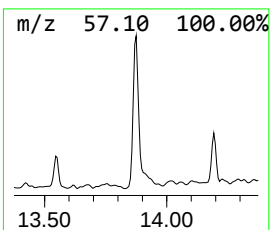
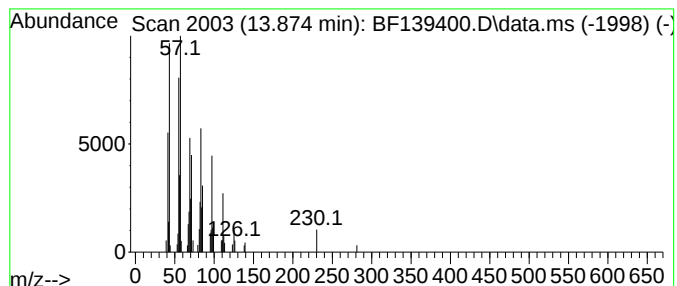
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.99 ng	71599	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
Data File : BF139400.D
Acq On : 17 Sep 2024 14:17
Operator : RC/JU
Sample : P3985-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

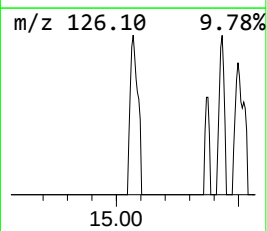
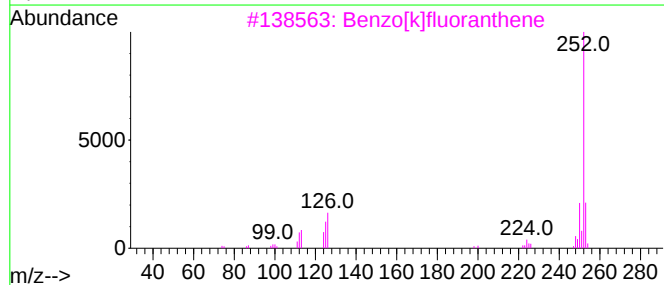
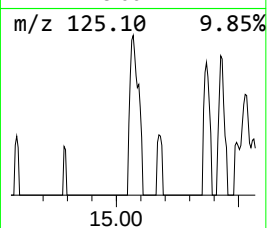
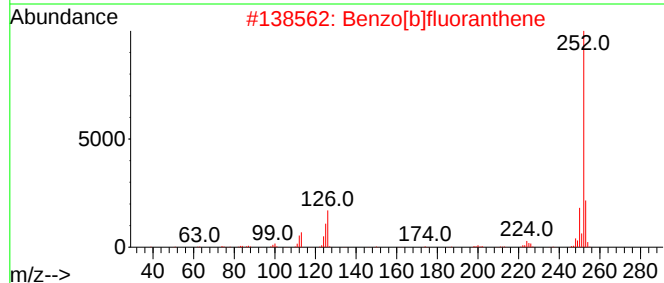
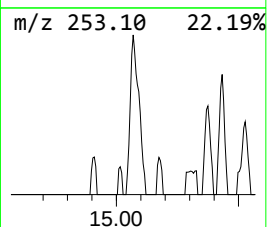
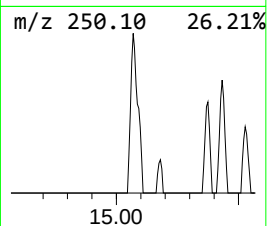
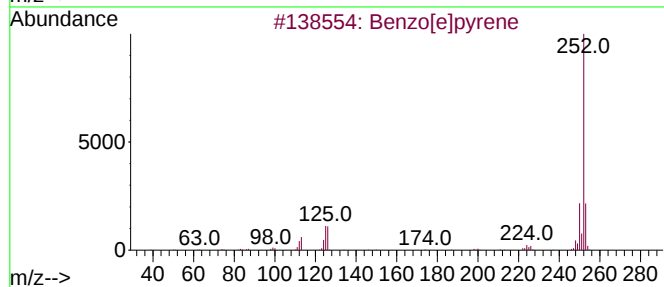
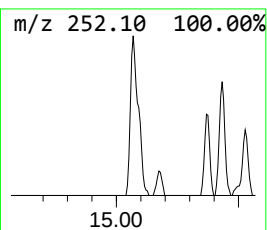
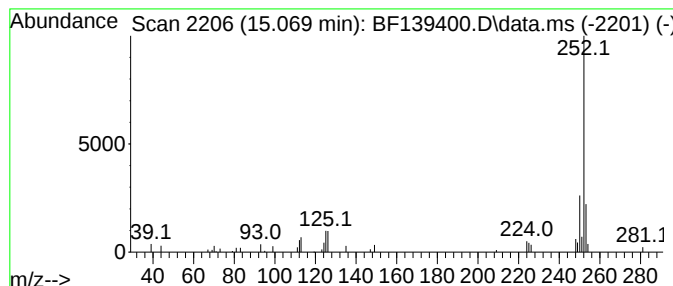
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.069	2.00 ng	28112	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	95
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	87
4			Benzo[a]pyrene	252	C20H12	000050-32-8	81
5			Perylene	252	C20H12	000198-55-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091724\
Data File : BF139400.D
Acq On : 17 Sep 2024 14:17
Operator : RC/JU
Sample : P3985-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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...	2.193	46.6	ng	980338	1	6.875	421112	20.0
unknown3.399	3.399	3.2	ng	67691	1	6.875	421112	20.0
2-Pentanone, 4-...	5.099	5.2	ng	109773	1	6.875	421112	20.0
1-Phenoxypropan...	8.469	2.2	ng	58738	2	8.157	527111	20.0
Benzophenone	10.622	5.5	ng	159264	3	9.910	575787	20.0
n-Hexadecanoic ...	11.916	3.8	ng	100954	4	11.392	529379	20.0
Pentadecafluoro...	13.874	4.0	ng	71599	5	14.027	358578	20.0
Benzo[e]pyrene	15.069	2.0	ng	28112	6	15.498	281004	20.0
Naphthalene, 1,...	17.145	2.9	ng	41340	6	15.498	281004	20.0