

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
 Data File : BF142452.D
 Acq On : 19 May 2025 15:33
 Operator : RC/JU
 Sample : Q2057-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-L

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-BF050525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142452.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	194	199	220	rBV	24933	61897	2.01%	0.333%
2	5.110	486	496	506	rBV	122237	177976	5.78%	0.959%
3	5.510	558	564	583	rBV	1200912	1586430	51.51%	8.544%
4	6.522	730	736	741	rBV	1254516	1629280	52.90%	8.775%
5	6.904	796	801	806	rBV	449014	543127	17.63%	2.925%
6	7.463	890	896	901	rBV	847838	1058482	34.37%	5.701%
7	8.186	1014	1019	1026	rBV	601044	743712	24.15%	4.006%
8	8.492	1066	1071	1082	rBV	86349	118996	3.86%	0.641%
9	9.257	1196	1201	1206	rBV	1790041	2178632	70.73%	11.734%
10	9.939	1312	1317	1322	rBV	676459	827357	26.86%	4.456%
11	10.028	1327	1332	1338	rVV	77732	117103	3.80%	0.631%
12	10.651	1433	1438	1445	rVB	67109	82581	2.68%	0.445%
13	10.727	1445	1451	1464	rBV	1282601	1697229	55.10%	9.141%
14	11.427	1564	1570	1577	rBV	850361	1152544	37.42%	6.207%
15	11.945	1651	1658	1671	rBV	237393	398484	12.94%	2.146%
16	12.639	1769	1776	1787	rBV	119188	175816	5.71%	0.947%
17	12.733	1787	1792	1805	rVV2	84667	147821	4.80%	0.796%
18	12.869	1808	1815	1820	rVB	86887	130326	4.23%	0.702%
19	13.010	1833	1839	1845	rBV	2318220	3080010	100.00%	16.588%
20	13.580	1932	1936	1945	rBV4	15569	33757	1.10%	0.182%
21	13.904	1987	1991	2002	rBV	109415	195308	6.34%	1.052%
22	14.063	2012	2018	2030	rBV	816946	1222622	39.70%	6.585%
23	14.533	2094	2098	2102	rBV3	22665	32561	1.06%	0.175%
24	14.698	2122	2126	2132	rVB3	20606	31296	1.02%	0.169%
25	15.115	2192	2197	2206	rBV	49571	118808	3.86%	0.640%
26	15.427	2246	2250	2256	rVB	29351	44361	1.44%	0.239%
27	15.492	2256	2261	2266	rBV	34773	59237	1.92%	0.319%
28	15.557	2266	2272	2284	rVB	563239	921409	29.92%	4.963%

Sum of corrected areas: 18567162

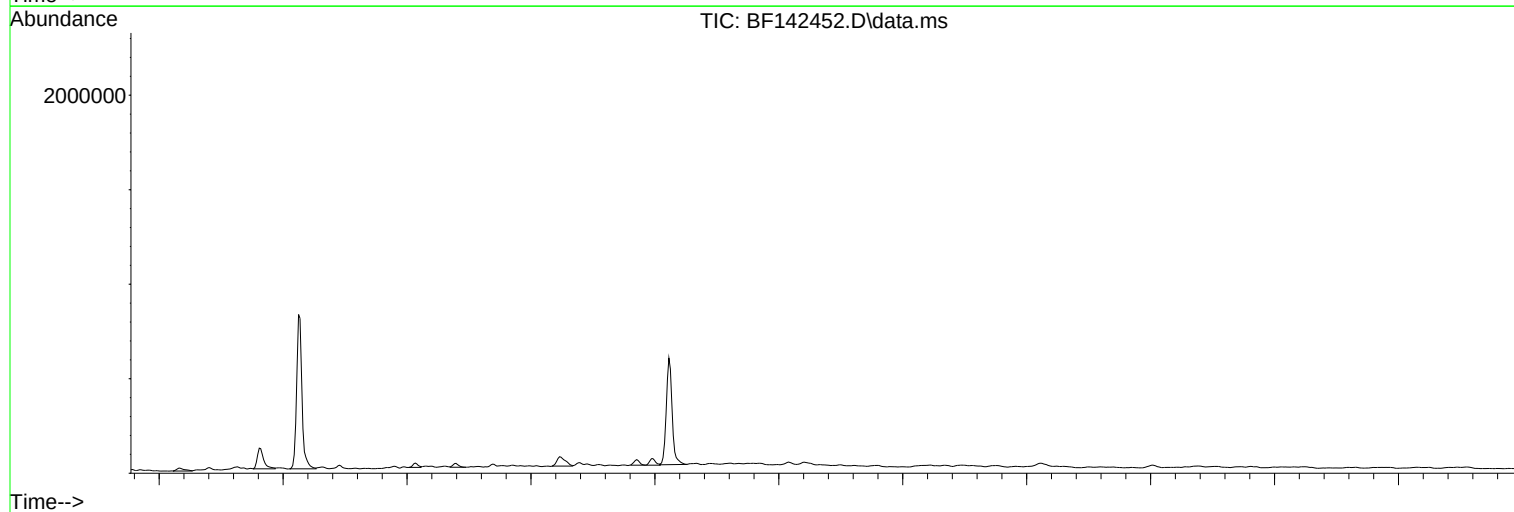
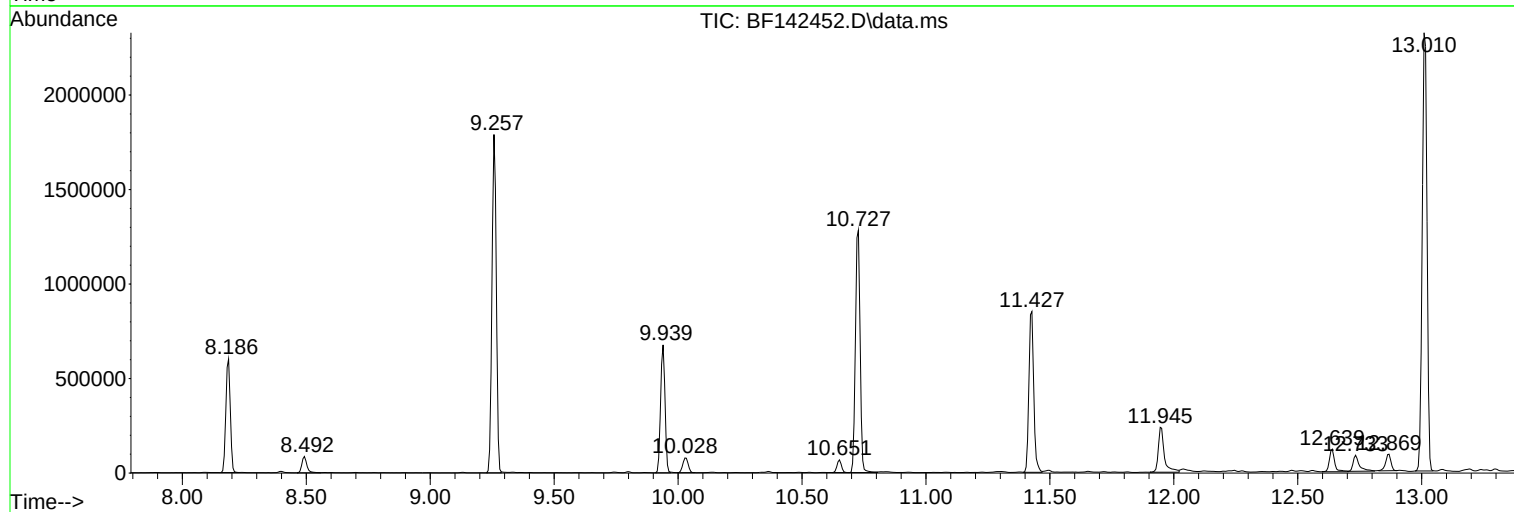
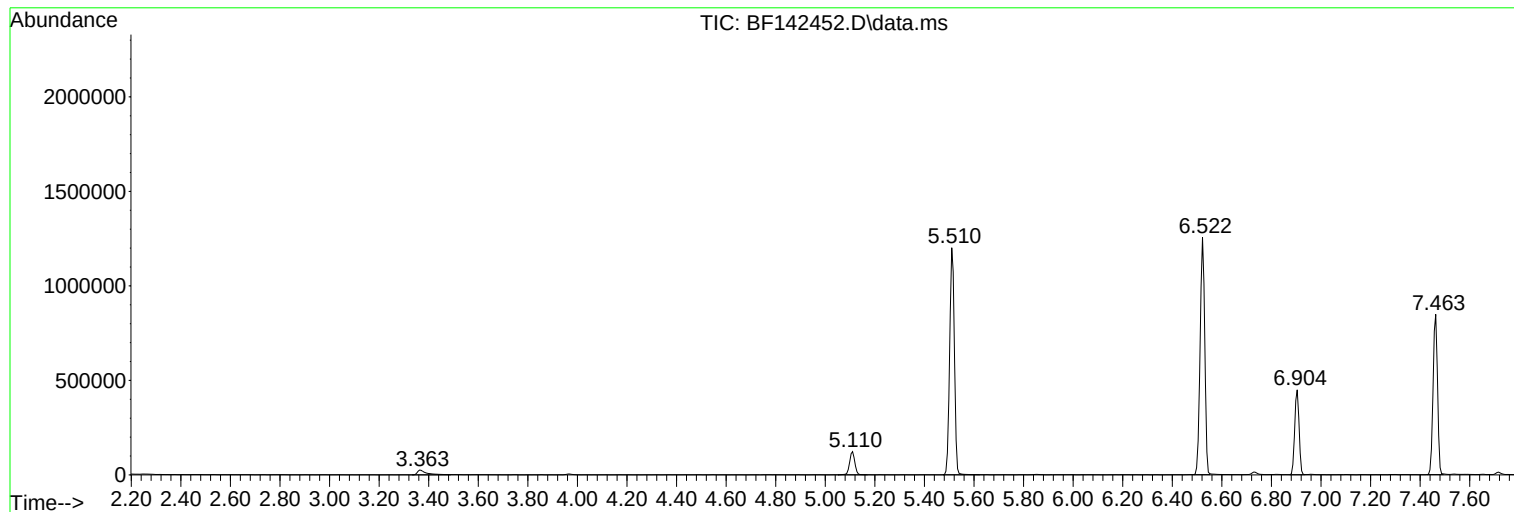
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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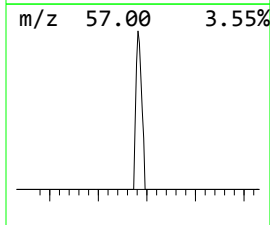
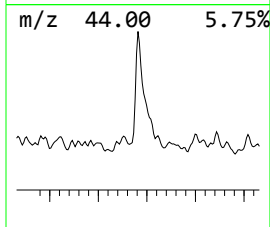
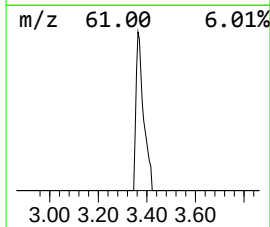
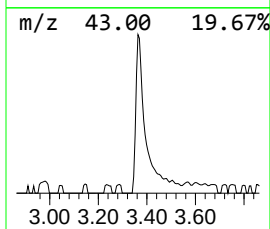
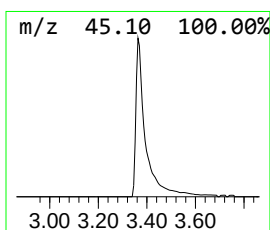
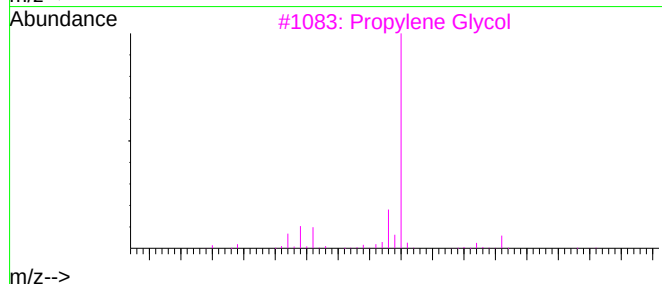
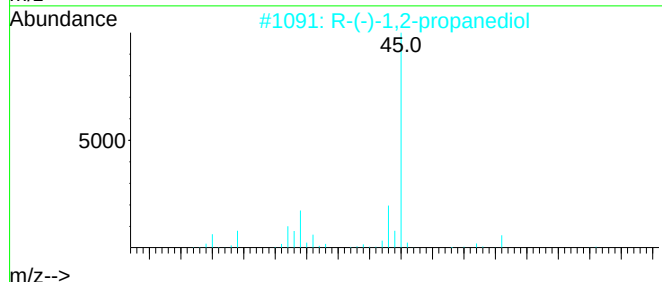
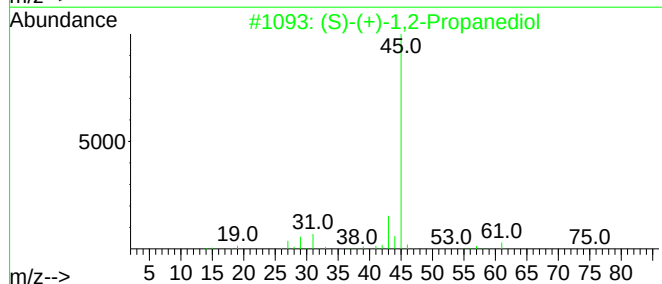
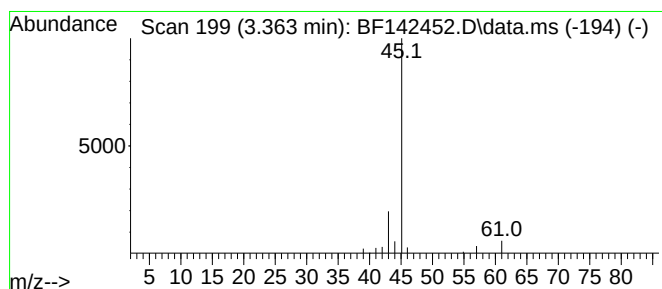
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	2.28 ng	61897	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Formamide	45	CH3NO	000075-12-7	5
5	2-Butanol, (R)-	74	C4H10O	014898-79-4	4



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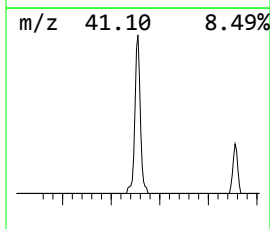
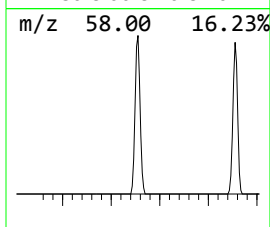
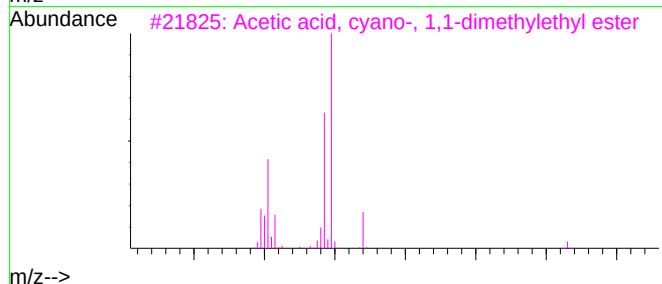
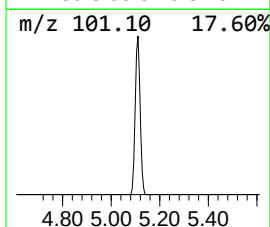
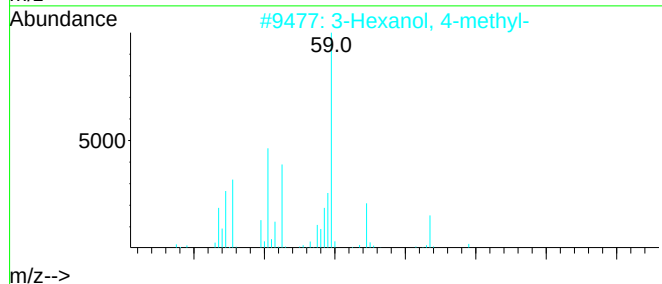
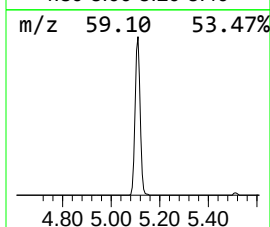
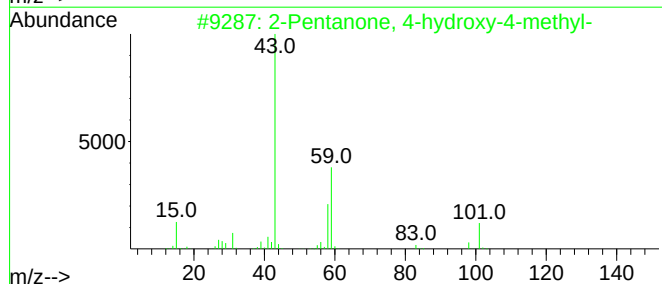
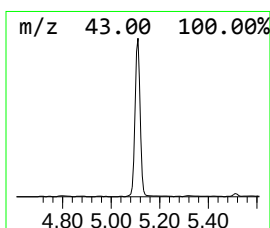
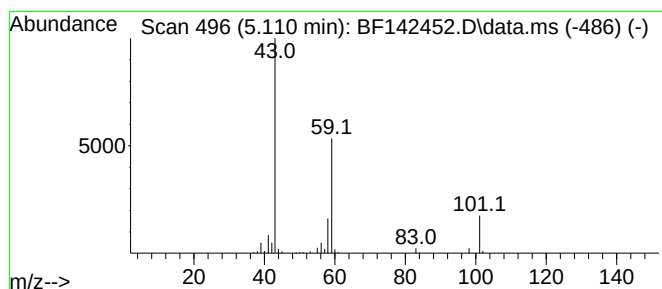
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	6.55 ng	177976	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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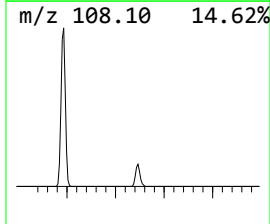
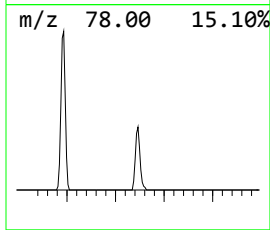
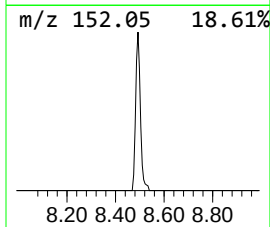
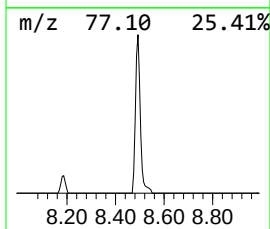
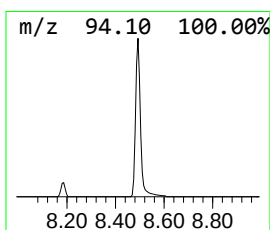
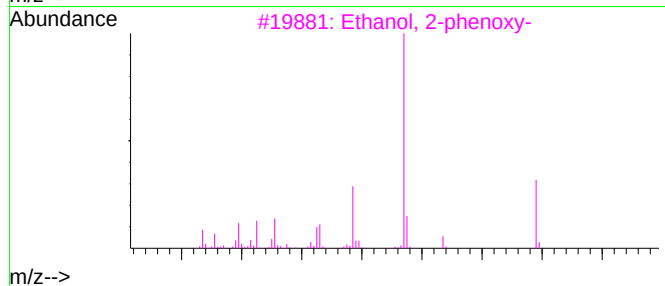
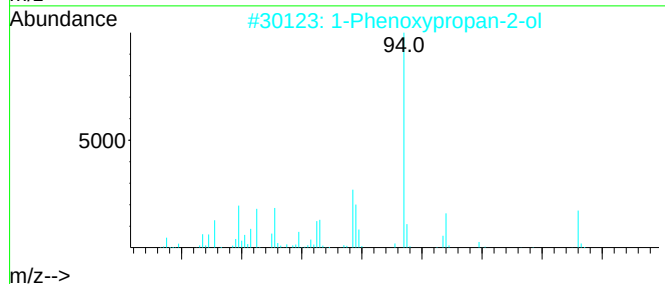
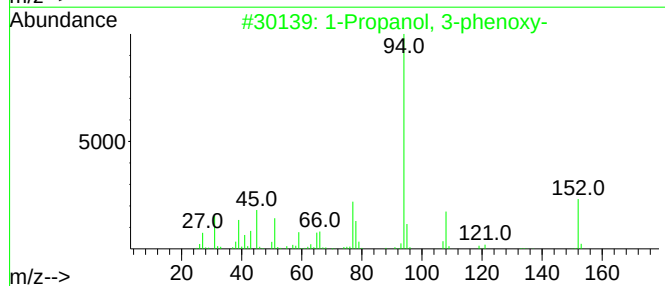
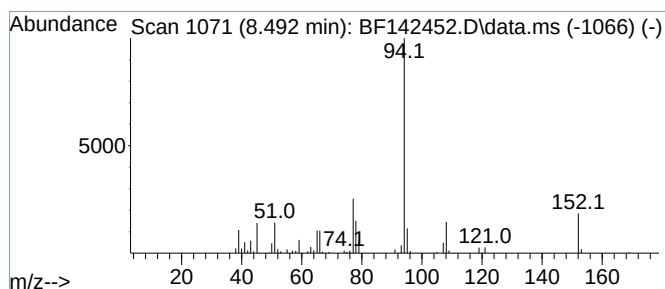
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol, 3-phenoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.492	3.20 ng	118996	Naphthalene-d8	8.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	97
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53



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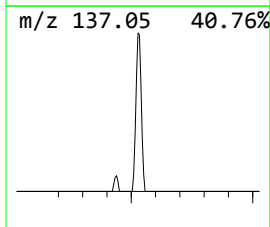
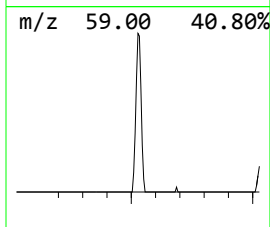
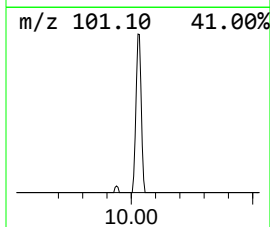
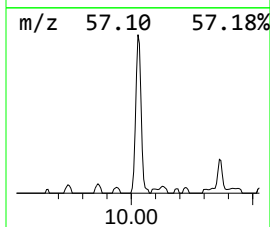
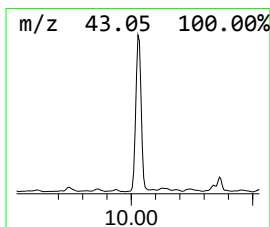
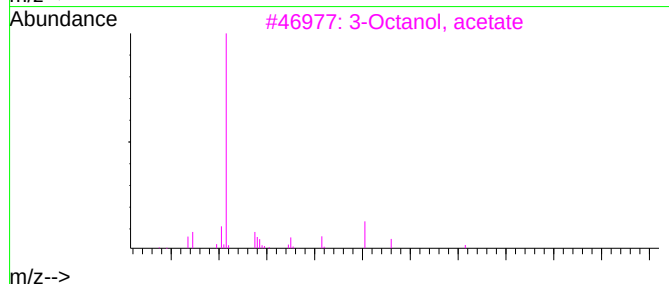
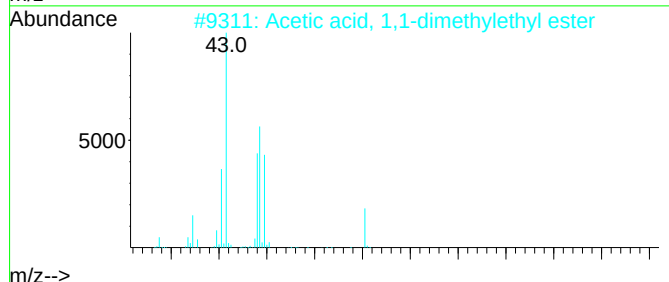
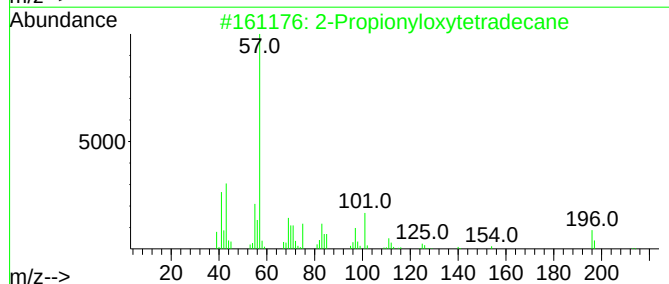
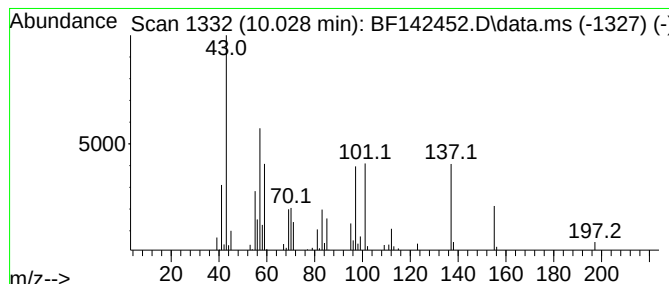
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.028 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.028	2.83 ng	117103	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propionyloxytetradecane	270	C17H34O2	1000245-62-7	27
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
3	3-Octanol, acetate	172	C10H20O2	004864-61-3	14
4	Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	12
5	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	11



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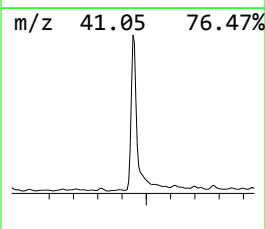
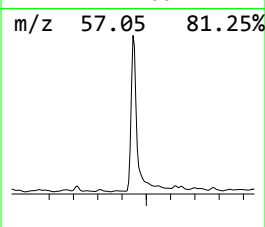
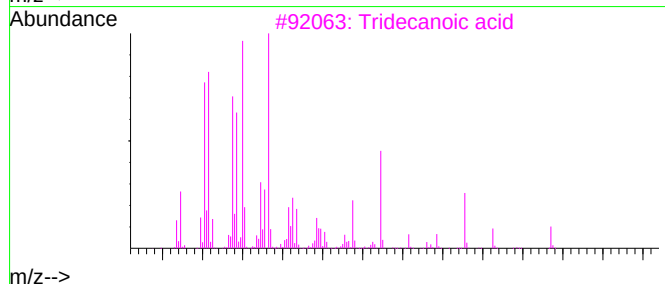
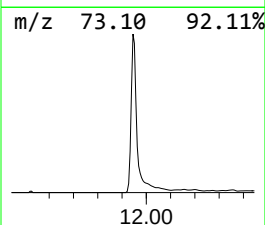
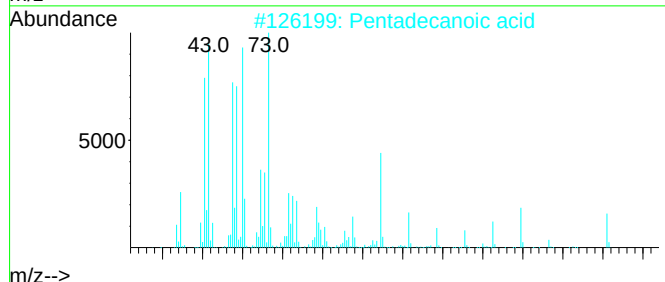
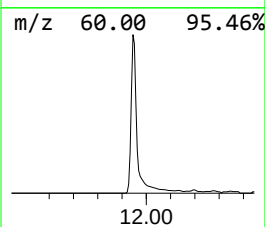
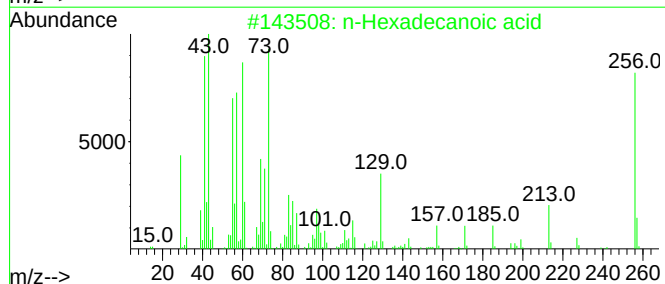
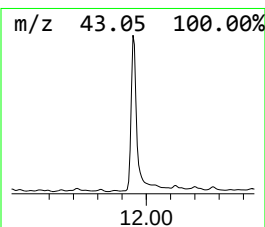
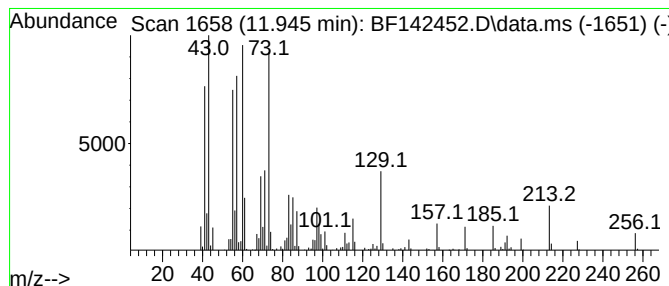
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.945	6.91 ng	398484	Phenanthrene-d10		11.427	
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	91
3	Tridecanoic acid		214	C13H26O2	000638-53-9	89
4	Dodecanoic acid		200	C12H24O2	000143-07-7	62
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	62



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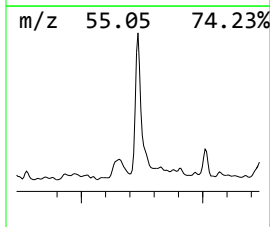
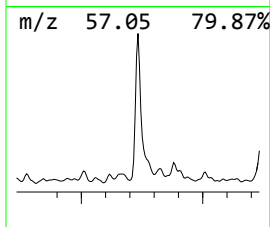
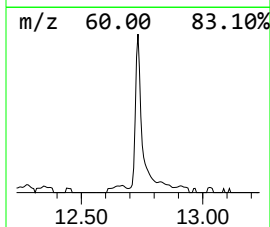
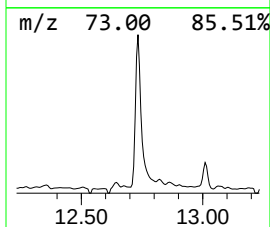
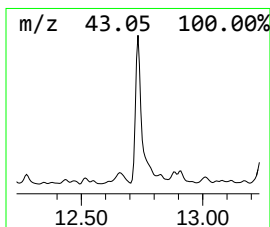
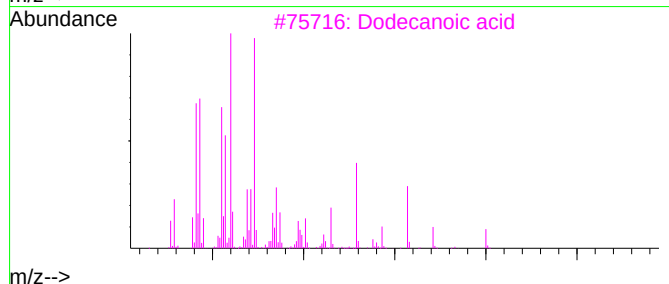
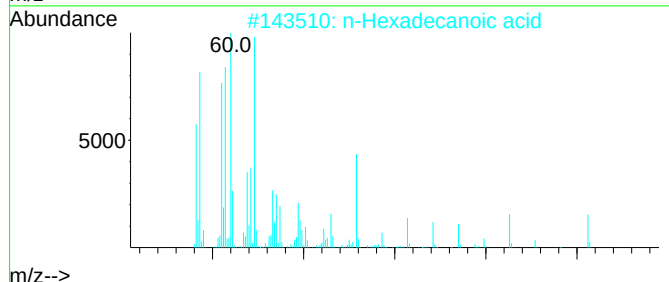
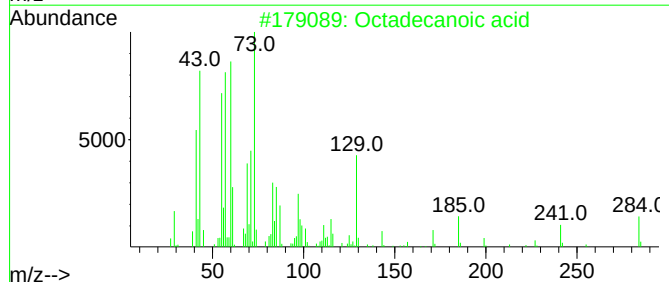
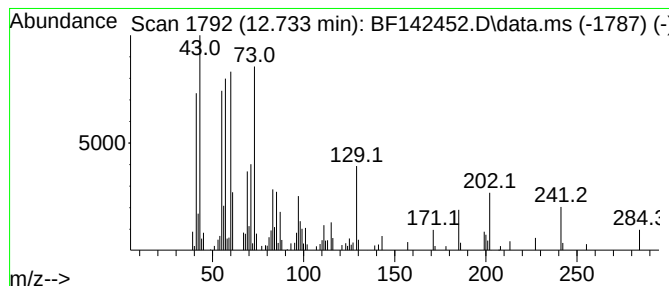
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.733	2.57 ng	147821	Phenanthrene-d10		11.427	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	81
3	Dodecanoic acid		200	C12H24O2	000143-07-7	78
4	n-Decanoic acid		172	C10H20O2	000334-48-5	78
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142452.D
Acq On : 19 May 2025 15:33
Operator : RC/JU
Sample : Q2057-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-L

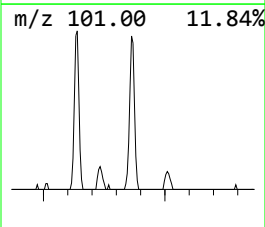
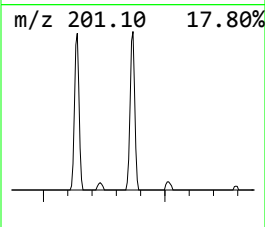
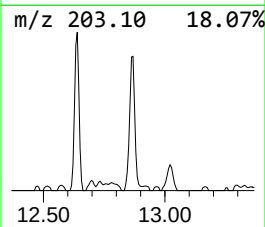
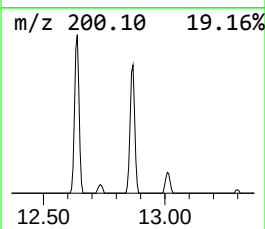
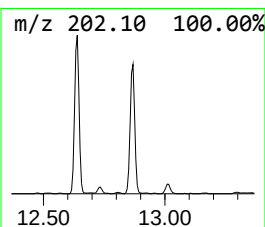
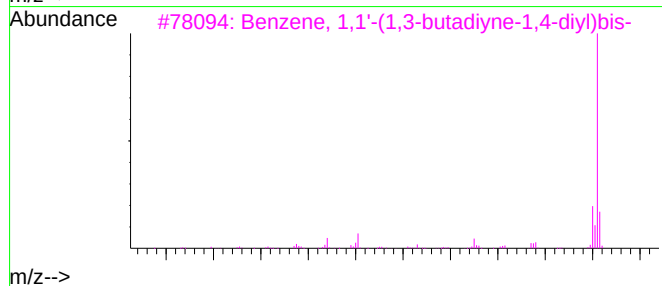
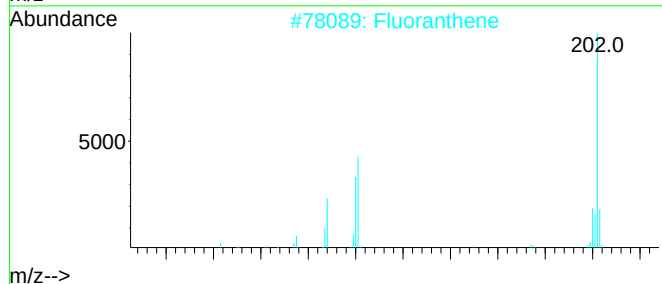
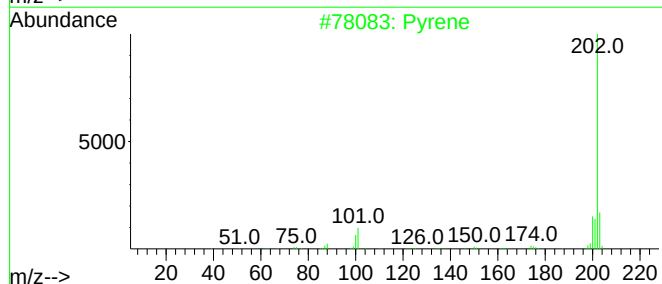
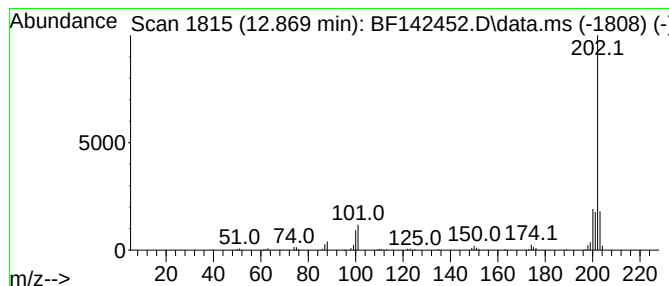
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.868	2.13 ng	130326	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	96
2	Fluoranthene	202	C16H10	000206-44-0	91
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
4	Succinic acid, di(4-cyanophenyl)...	320	C18H12N2O4	1000360-71-2	28
5	Benzaldehyde, 2,6-difluoro-3,4-d...	202	C9H8F2O3	152434-99-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142452.D
Acq On : 19 May 2025 15:33
Operator : RC/JU
Sample : Q2057-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-L

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

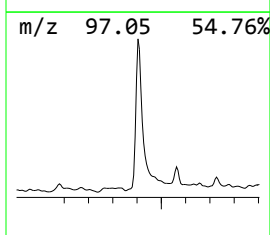
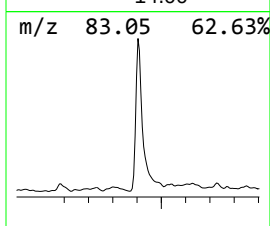
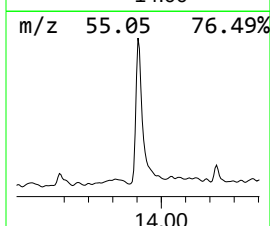
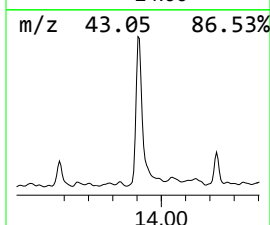
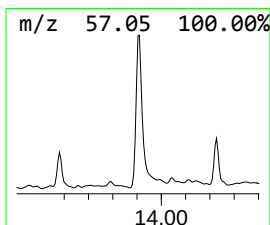
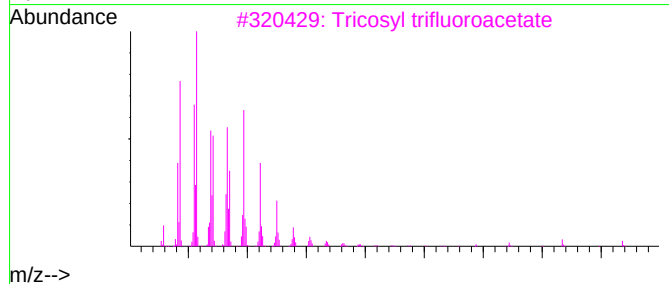
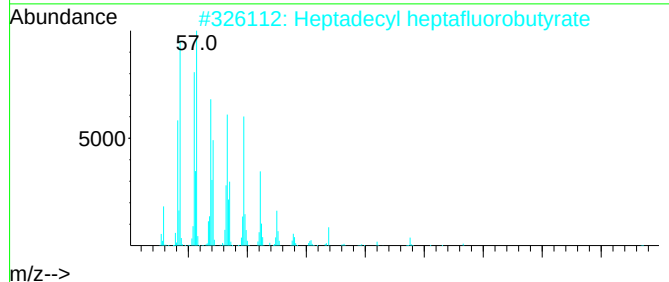
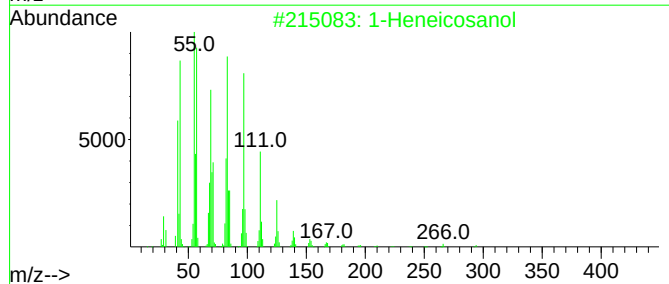
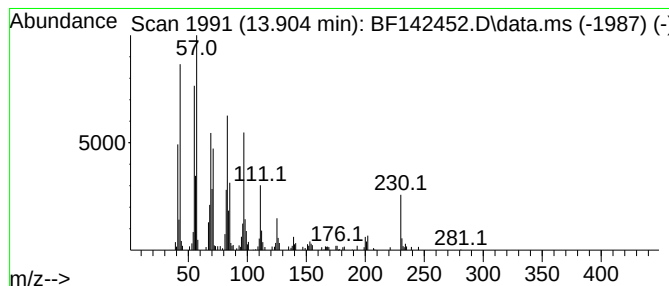
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.19 ng	195308	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	93
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142452.D
Acq On : 19 May 2025 15:33
Operator : RC/JU
Sample : Q2057-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

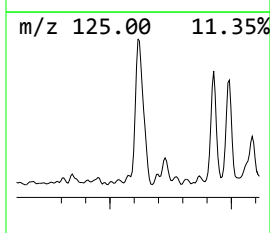
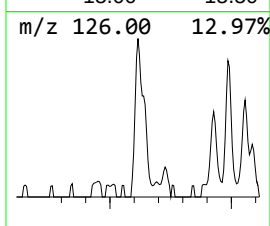
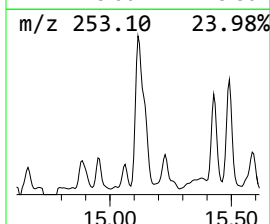
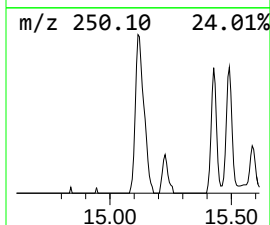
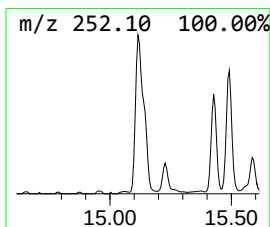
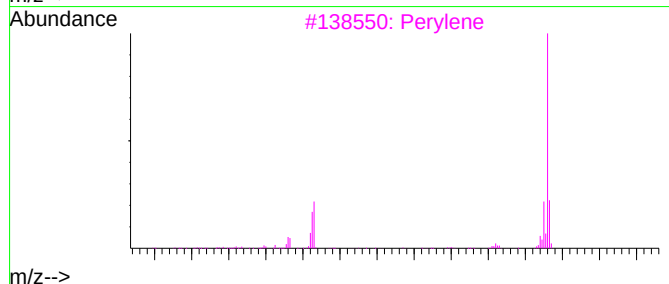
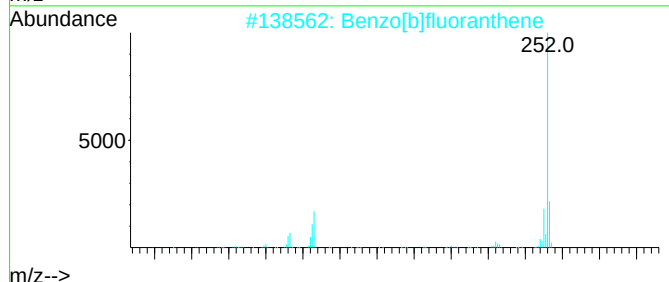
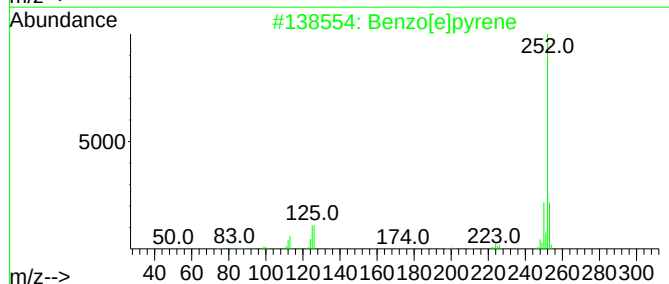
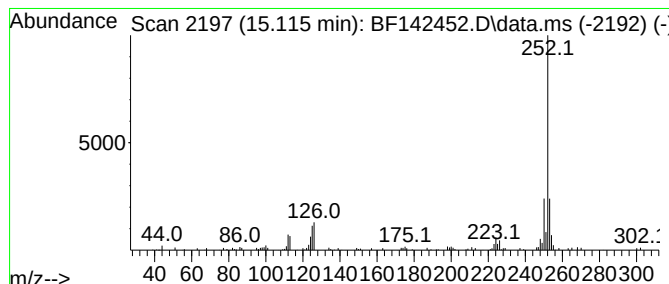
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.115	2.58 ng	118808	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Perylene	252	C20H12	000198-55-0	90
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142452.D
Acq On : 19 May 2025 15:33
Operator : RC/JU
Sample : Q2057-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-L

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.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
(S)-(+)-1,2-Pro...	3.363	2.3	ng	61897	1	6.904	543127	20.0
2-Pentanone, 4-...	5.110	6.5	ng	177976	1	6.904	543127	20.0
1-Propanol, 3-p...	8.492	3.2	ng	118996	2	8.186	743712	20.0
unknown10.028	10.028	2.8	ng	117103	3	9.939	827357	20.0
n-Hexadecanoic ...	11.945	6.9	ng	398484	4	11.427	1152540	20.0
Octadecanoic acid	12.733	2.6	ng	147821	4	11.427	1152540	20.0
Benzene, 1,1'-(...	12.868	2.1	ng	130326	5	14.063	1222620	20.0
1-Heneicosanol	13.904	3.2	ng	195308	5	14.063	1222620	20.0
Benzo[e]pyrene	15.115	2.6	ng	118808	6	15.557	921409	20.0