LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138997.D
Acq On : 14 Aug 2024 16:42
Operator : RC/JU
Sample : P3548-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200036

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138997.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.369	213	217	234	rBV	11226	39042	4.19%	0.551%
2	5.057	499	504	524	rVB	38543	60528	6.50%	0.854%
3	5.469	569	574	597	rBV	600456	857770	92.05%	12.106%
4	6.481	741	746	766	rBV	694835	931802	100.00%	13.151%
5	6.687	774	781	787	rBV	6871	14501	1.56%	0.205%
6	6.834	801	806	815	rVB	199542	242374	26.01%	3.421%
7	7.398	897	902	920	rBV	414572	543892	58.37%	7.676%
8	7.663	943	947	954	rBV2	7488	12130	1.30%	0.171%
9	8.116	1019	1024	1042	rVB	247633	317215	34.04%	4.477%
10	8.434	1073	1078	1091	rBV	38121	61962	6.65%	0.874%
11	9.187	1201	1206	1211	rBV	583872	706077	75.78%	9.965%
12	9.863	1317	1321	1325	rBV	229520	291142	31.25%	4.109%
13	9.898	1325	1327	1332	rVB	24152	26064	2.80%	0.368%
14	9.957	1332	1337	1345	rBV	19396	29708	3.19%	0.419%
15	10.075	1353	1357	1361	rBV	9163	10135	1.09%	0.143%
16	10.416	1410	1415	1421	rVB	15639	18705	2.01%	0.264%
17	10.657	1451	1456	1469	rBV	291251	377224	40.48%	5.324%
18	10.781	1469	1477	1486	rVB2	7319	15515	1.67%	0.219%
19	11.351	1569	1574	1577	rBV	178341	261264	28.04%	3.687%
20	11.375	1577	1578	1584	rVV	142658	134530	14.44%	1.899%
21	11.433	1584	1588	1593	rVB	25340	31965	3.43%	0.451%
22	11.592	1610	1615	1619	rBV2	12187	15675	1.68%	0.221%
23	11.857	1656	1660	1662	rBV	10362	13427	1.44%	0.189%
24	11.886	1662	1665	1670	rVB	15476	19844	2.13%	0.280%
25	11.969	1675	1679	1687	rVB	19374	32720	3.51%	0.462%
26	12.569	1776	1781	1787	rBV	158969	197062	21.15%	2.781%
27	12.798	1813	1820	1826	rBV	124538	186426	20.01%	2.631%
28	12.933	1838	1843	1847	rBV	395618	484345	51.98%	6.836%
29	13.016	1852	1857	1861	rBV3	6299	11216	1.20%	0.158%
30	13.127	1868	1876	1880	rVB	15189	25952	2.79%	0.366%
31	13.192	1883	1887	1890	rBV	9188	11332	1.22%	0.160%
32	13.233	1890	1894	1900	rVB3	9075	16069	1.72%	0.227%
33	13.645	1960	1964	1968	rBV	9978	11522	1.24%	0.163%
34	13.751	1976	1982	1984	rBV	12665	20015	2.15%	0.282%
35	13.804	1988	1991	1995	rVV2	7896	16400	1.76%	0.231%
36	13.851	1995	1999	2006	rVB	18666	31987	3.43%	0.451%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138997.D
Acq On : 14 Aug 2024 16:42
Operator : RC/JU
Sample : P3548-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200036

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.963	2013	2018	2019	rBV	56718	73429	7.88%	1.036%
38	13.992	2019	2023	2036	rVV2	211642	415965	44.64%	5.871%
39	14.104	2038	2042	2045	rVB	10335	12169	1.31%	0.172%
40	14.386	2085	2090	2093	rVB	9086	12245	1.31%	0.173%
41	14.816	2160	2163	2167	rVB	8846	11683	1.25%	0.165%
42	14.886	2171	2175	2183	rBV4	5448	9559	1.03%	0.135%
43	15.039	2195	2201	2212	rBV	60840	140817	15.11%	1.987%
44	15.145	2215	2219	2226	rVB	8818	13839	1.49%	0.195%
45	15.339	2247	2252	2258	rVB	25910	38423	4.12%	0.542%
46	15.404	2258	2263	2268	rBV	37534	56302	6.04%	0.795%
47	15.463	2268	2273	2278	rBV	96923	154662	16.60%	2.183%
48	16.939	2518	2524	2532	rVB2	16192	35806	3.84%	0.505%
49	17.386	2594	2600	2607	rBV2	10868	23394	2.51%	0.330%
50	17.651	2635	2645	2649	rBV10	3127	9814	1.05%	0.139%

Sum of corrected areas: 7085644

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
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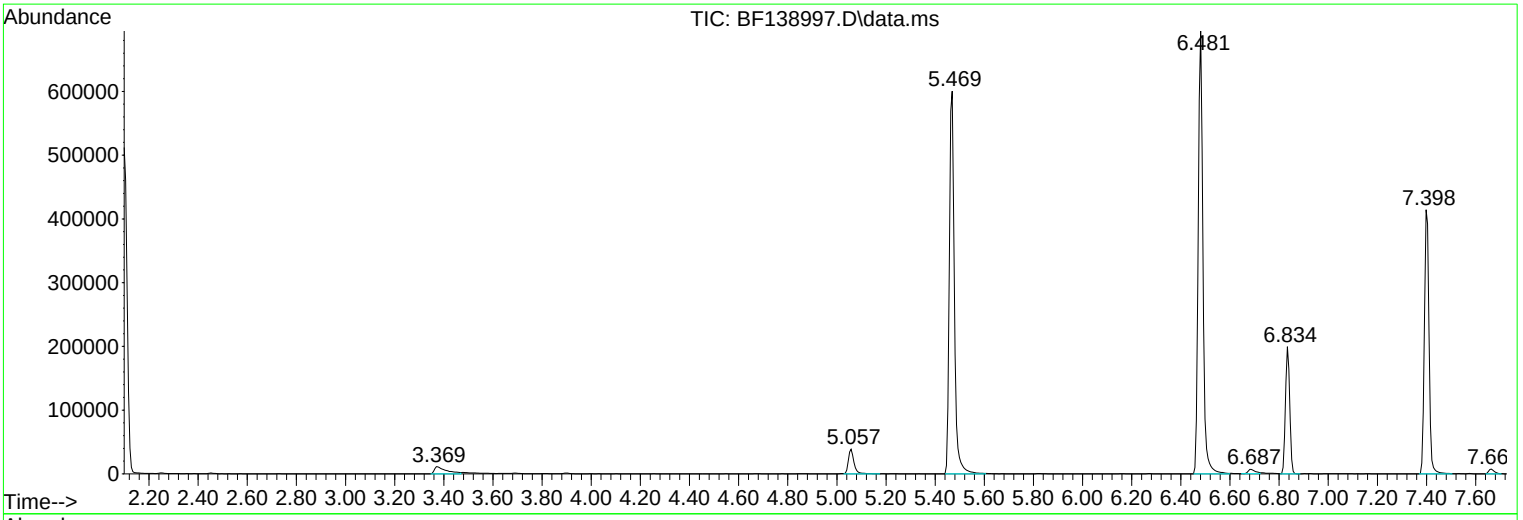
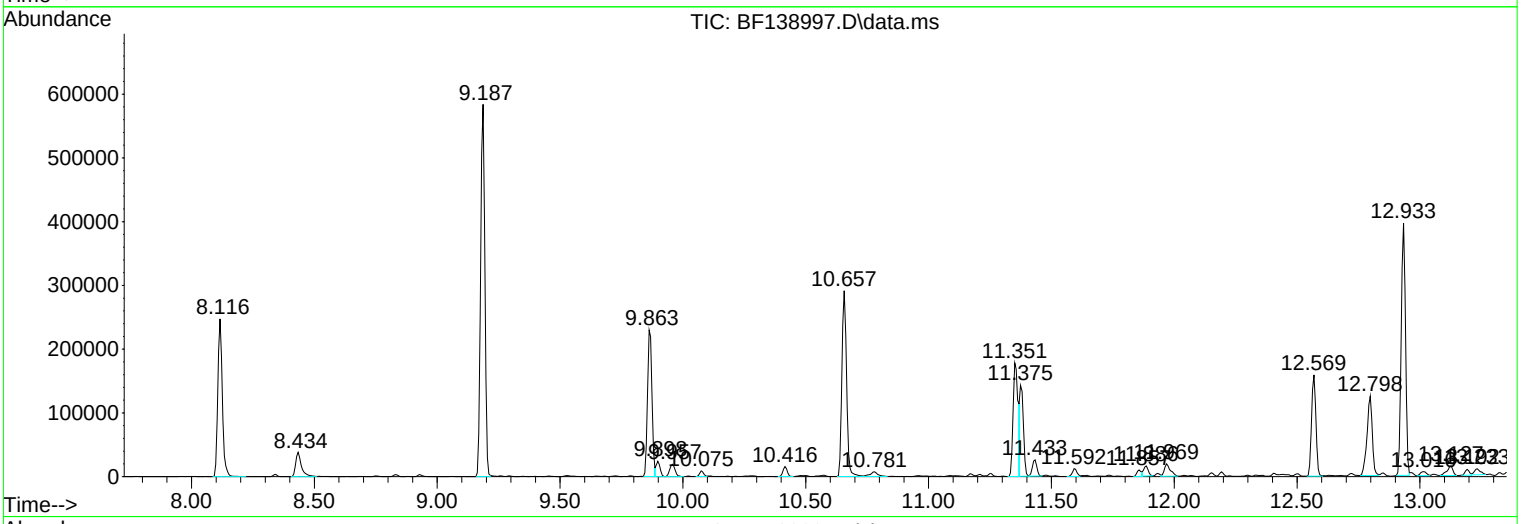
Misc :
ALS Vial : 11 Sample Multiplier: 1

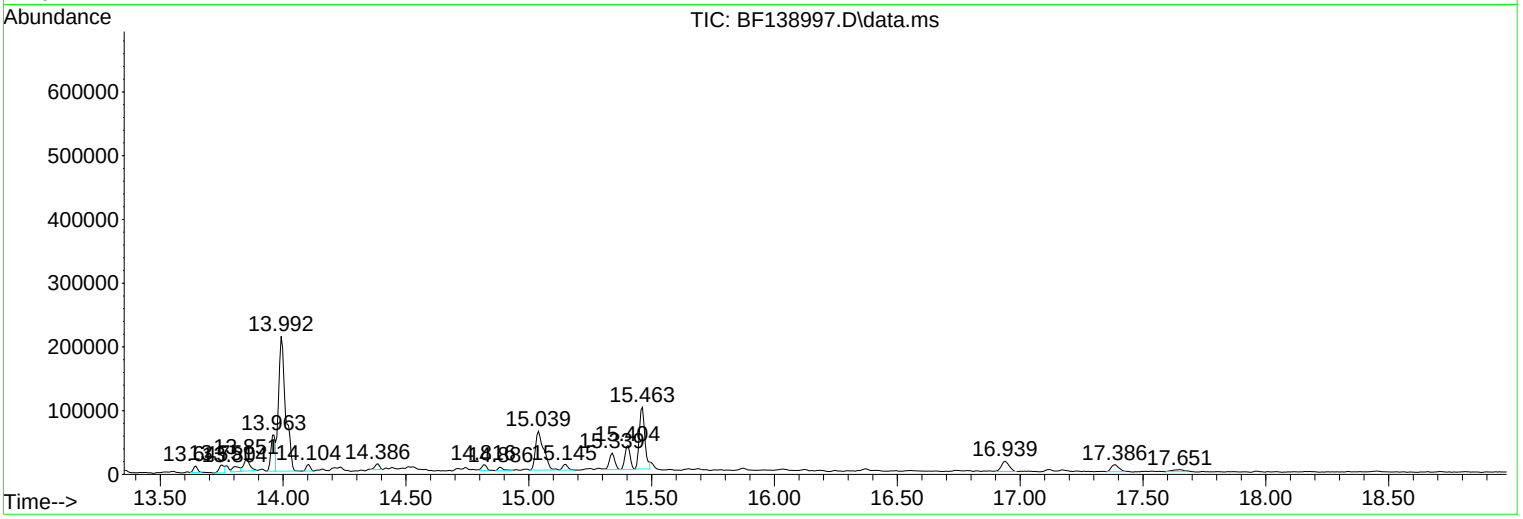
Instrument :
BNA_F
ClientSampleId :
RBR200036

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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\BF081424\
Data File : BF138997.D
Acq On : 14 Aug 2024 16:42
Operator : RC/JU
Sample : P3548-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200036

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

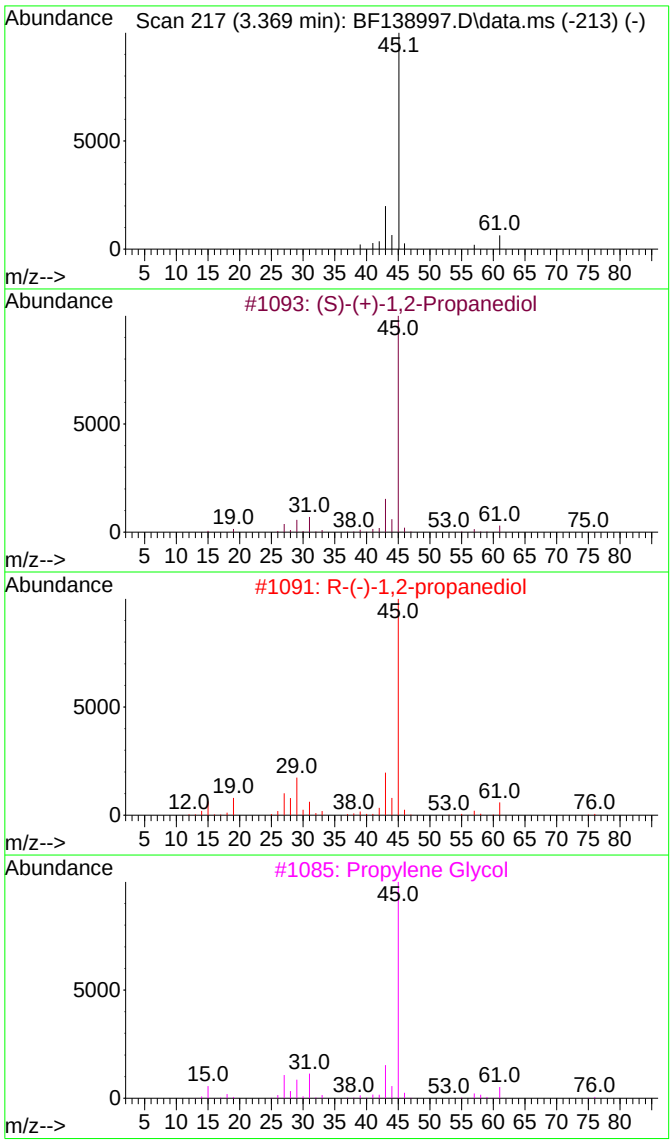
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

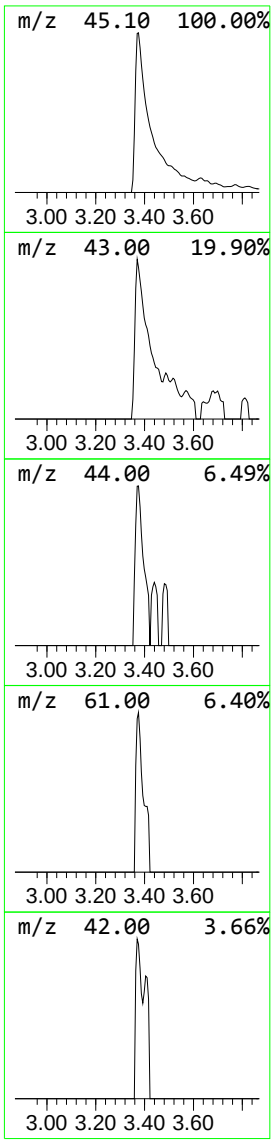
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.369	3.22 ng	39042	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138997.D
Acq On : 14 Aug 2024 16:42
Operator : RC/JU
Sample : P3548-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200036

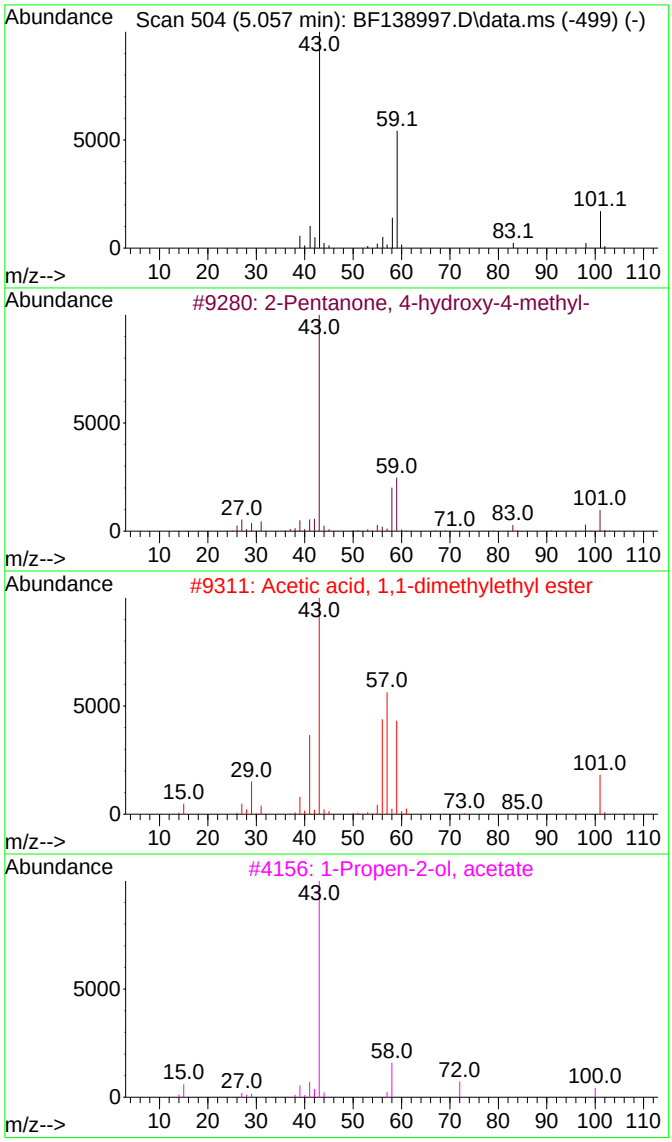
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

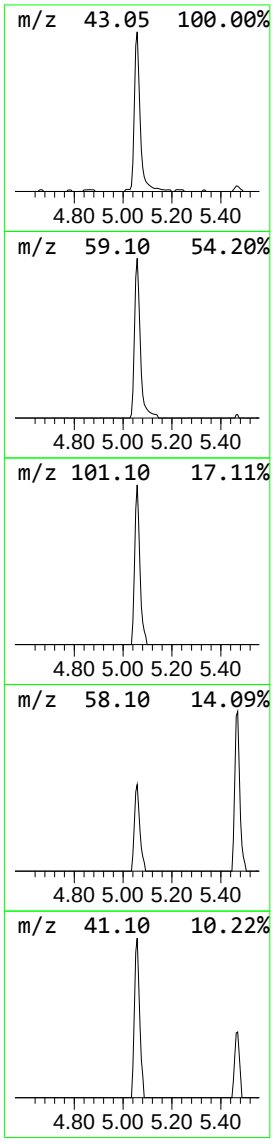
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	4.99 ng	60528	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138997.D
Acq On : 14 Aug 2024 16:42
Operator : RC/JU
Sample : P3548-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200036

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

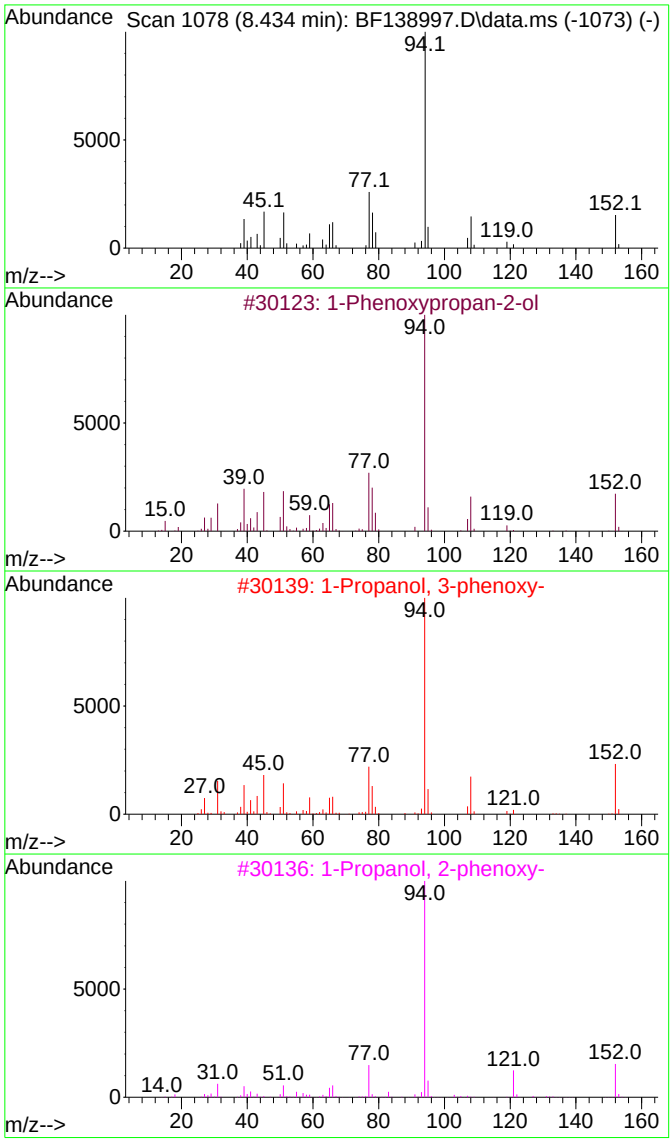
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

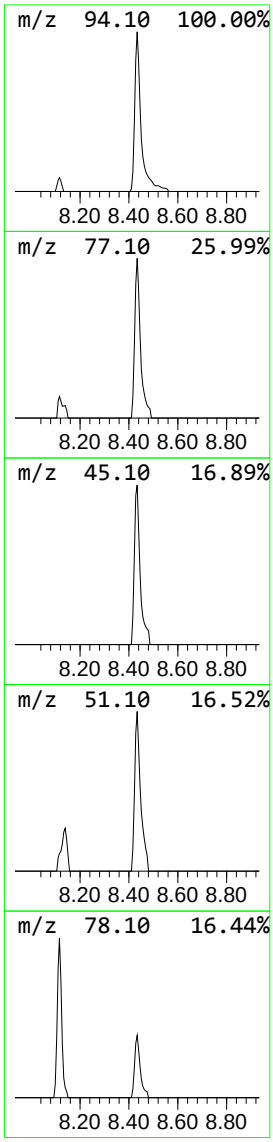
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	3.91 ng	61962	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53
5	Benzene, propoxy-	136	C9H12O	000622-85-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138997.D
Acq On : 14 Aug 2024 16:42
Operator : RC/JU
Sample : P3548-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200036

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

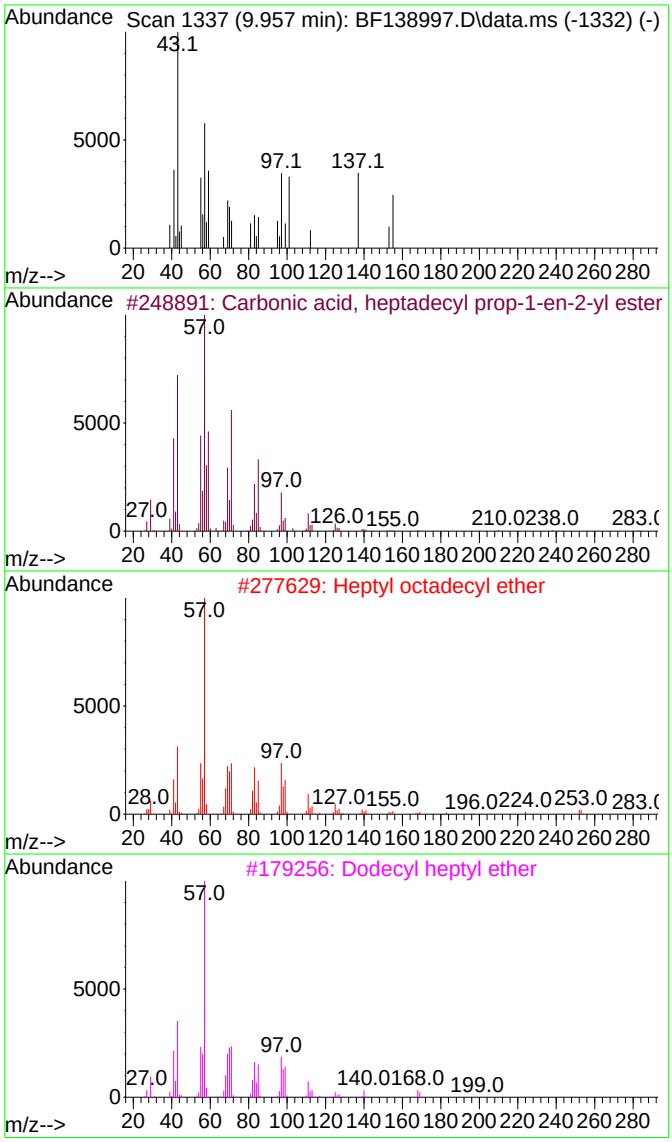
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

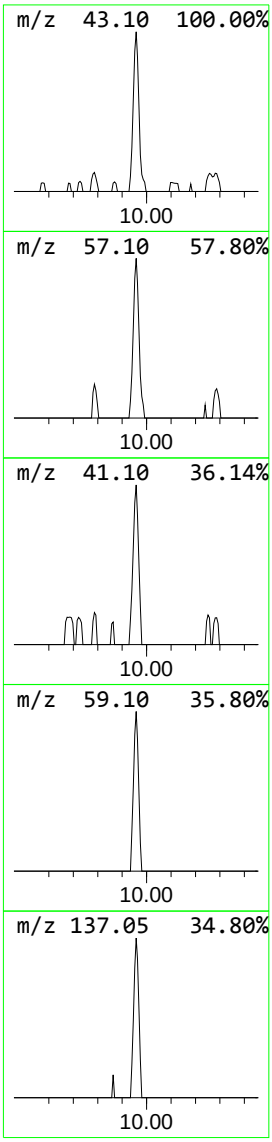
****

Peak Number 4 unknown9.957 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.957	2.04 ng	29708	Acenaphthene-d10	9.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, heptadecyl prop-1...	340	C21H40O3	1000382-90-2	10
2	Heptyl octadecyl ether	368	C25H52O	1000406-39-5	10
3	Dodecyl heptyl ether	284	C19H40O	1010406-39-2	10
4	5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	10
5	Heptyl octacosyl ether	509	C35H72O	1000406-40-0	10





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Acq On : 14 Aug 2024 16:42
Operator : RC/JU
Sample : P3548-03
Misc :
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Instrument :
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ClientSampleId :
RBR200036

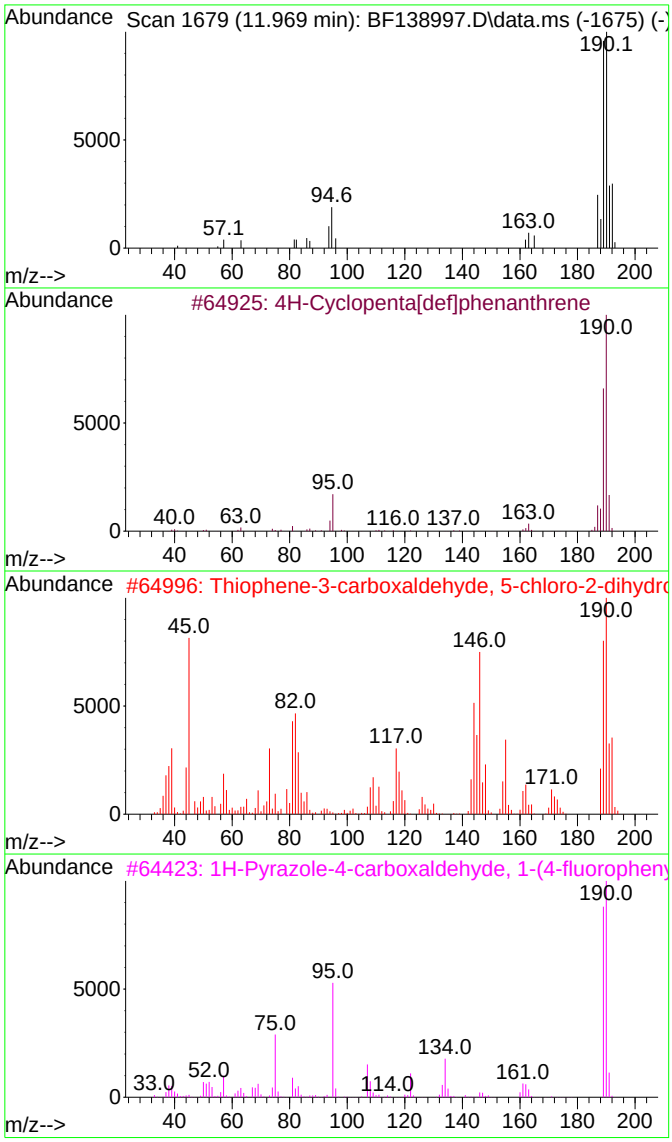
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

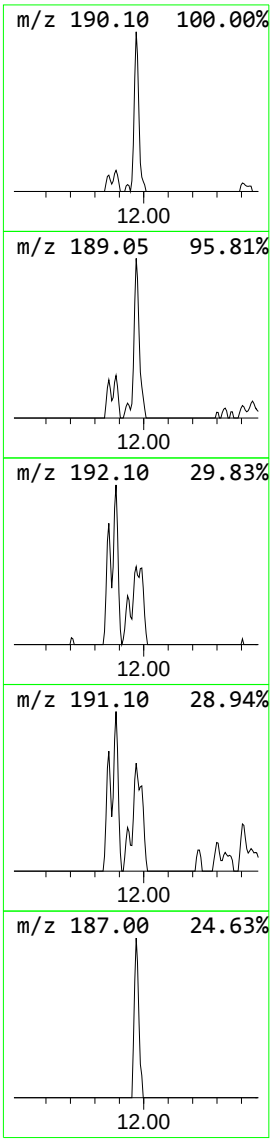
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.50 ng	32720	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
3	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	42
4	Methyl diselenide	190	C2H6Se2	007101-31-7	38
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36





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Operator : RC/JU
Sample : P3548-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200036

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

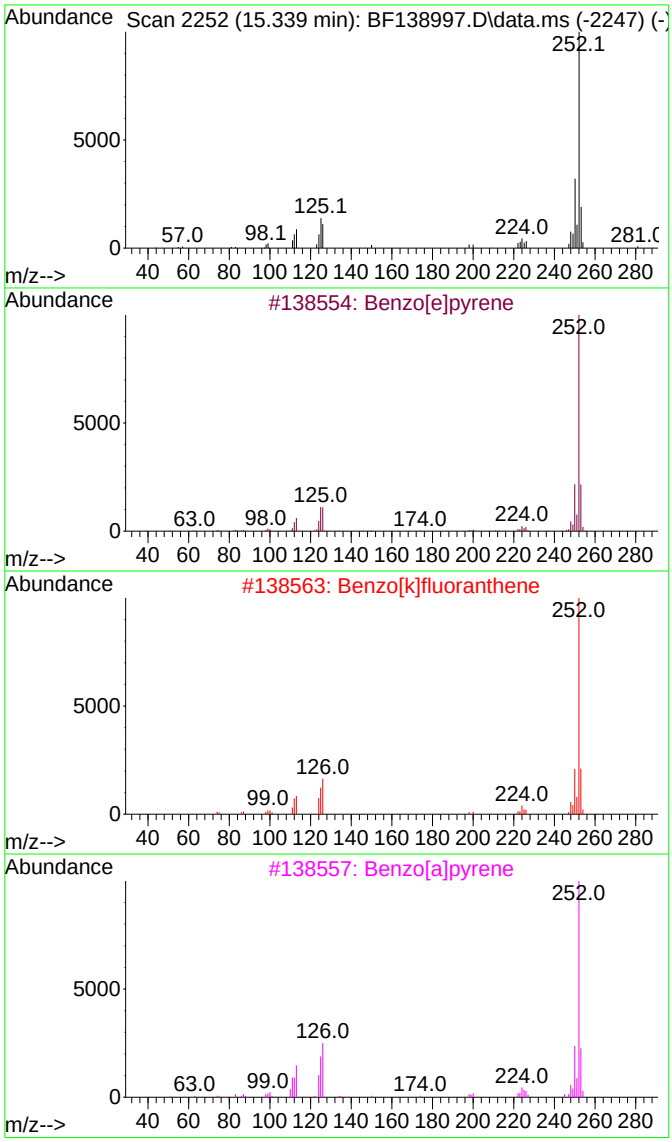
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

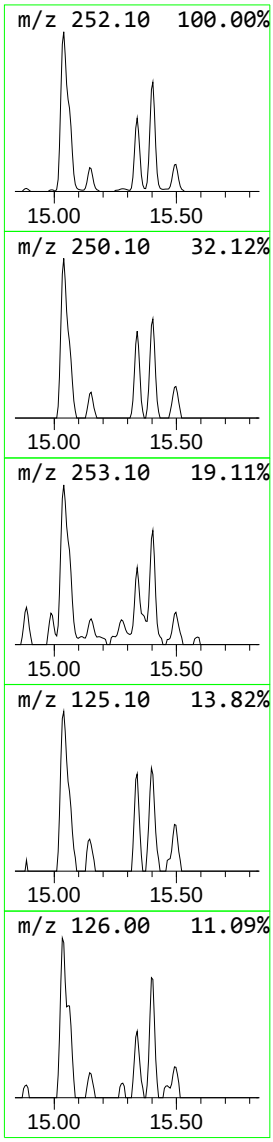
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	4.97 ng	38423	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[a]pyrene	252	C20H12	000050-32-8	95
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138997.D
Acq On : 14 Aug 2024 16:42
Operator : RC/JU
Sample : P3548-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200036

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(S)-(+)-1,2-Pro...	3.369	3.2	ng	39042	1	6.834	242374	20.0
2-Pentanone, 4-...	5.057	5.0	ng	60528	1	6.834	242374	20.0
1-Phenoxypropan...	8.434	3.9	ng	61962	2	8.116	317215	20.0
unknown9.957	9.957	2.0	ng	29708	3	9.863	291142	20.0
4H-Cyclopenta[d...	11.969	2.5	ng	32720	4	11.351	261264	20.0
Benzo[e]pyrene	15.339	5.0	ng	38423	6	15.463	154662	20.0