LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	28	rVB	4344637	5606539	54.79%	6.851%
2	3.463	223	234	244	rBV	428765	1134288	11.08%	1.386%
3	5.122	512	516	521	rVB	464324	486418	4.75%	0.594%
4	5.516	578	583	586	rBV	6714836	7337676	71.70%	8.967%
5	6.522	748	754	757	rBV	6297745	7248618	70.83%	8.858%
6	6.716	784	787	793	rBV	817352	623488	6.09%	0.762%
7	6.892	813	817	820	rBV	3059864	2393332	23.39%	2.925%
8	7.457	907	913	916	rBV	4767430	4803721	46.94%	5.870%
9	7.704	951	955	958	rBV	284866	208319	2.04%	0.255%
10	8.175	1030	1035	1037	rBV	3443237	3128948	30.58%	3.824%
11	8.386	1066	1071	1074	rBV	148713	111504	1.09%	0.136%
12	8.480	1083	1087	1097	rBV	873544	771203	7.54%	0.942%
13	9.245	1213	1217	1220	rBV	9256008	8432656	82.40%	10.305%
14	9.504	1257	1261	1265	rBV4	111240	113403	1.11%	0.139%
15	9.780	1305	1308	1312	rVB	120504	116533	1.14%	0.142%
16	9.922	1329	1332	1336	rBV	3686229	3125416	30.54%	3.819%
17	10.027	1344	1350	1354	rBV	7131271	10233500	100.00%	12.505%
18	10.469	1422	1425	1429	rVB	132614	111765	1.09%	0.137%
19	10.710	1462	1466	1469	rBV	4713556	3995703	39.05%	4.883%
20	11.410	1581	1585	1587	rBV	2975222	2494302	24.37%	3.048%
21	11.433	1587	1589	1592	rVV	1065306	818833	8.00%	1.001%
22	11.480	1595	1597	1600	rVB	221603	170966	1.67%	0.209%
23	11.633	1618	1623	1629	rBV	95469	139781	1.37%	0.171%
24	11.798	1648	1651	1654	rBV	163623	139254	1.36%	0.170%
25	11.910	1666	1670	1671	rBV	187801	160401	1.57%	0.196%
26	11.933	1671	1674	1679	rVB	645932	562276	5.49%	0.687%
27	12.016	1685	1688	1691	rBV2	229804	262415	2.56%	0.321%
28	12.457	1759	1763	1766	rBV	204396	202087	1.97%	0.247%
29	12.492	1766	1769	1770	rVV2	129439	151253	1.48%	0.185%
30	12.510	1770	1772	1775	rVV2	195633	175717	1.72%	0.215%
31	12.615	1787	1790	1794	rVB	1017813	876262	8.56%	1.071%
32	12.715	1804	1807	1809	rBV2	174561	153199	1.50%	0.187%
33	12.845	1823	1829	1835	rBV	1036097	1077280	10.53%	1.316%
34	12.904	1835	1839	1842	rVB3	75677	103587	1.01%	0.127%
35	12.992	1850	1854	1857	rBV	6729503	5669349	55.40%	6.928%
36	13.062	1862	1866	1870	rBV2	104794	150993	1.48%	0.185%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.174	1882	1885	1888	rVB	196442	186242	1.82%	0.228%
38	13.239	1889	1896	1899	rBV2	136748	190292	1.86%	0.233%
39	13.280	1899	1903	1905	rVV2	148741	142610	1.39%	0.174%
40	13.368	1916	1918	1921	rVB	135095	109117	1.07%	0.133%
41	13.398	1921	1923	1927	rVB	120718	111671	1.09%	0.136%
42	13.680	1968	1971	1976	rVB	86040	105344	1.03%	0.129%
43	13.792	1985	1990	1993	rBV3	121797	180681	1.77%	0.221%
44	13.898	2004	2008	2017	rBV4	190679	354820	3.47%	0.434%
45	14.045	2027	2033	2035	rBV2	2264187	2592541	25.33%	3.168%
46	14.068	2035	2037	2043	rVB	491663	428606	4.19%	0.524%
47	14.139	2044	2049	2054	rBV3	266936	359367	3.51%	0.439%
48	14.427	2094	2098	2101	rBV	145581	148908	1.46%	0.182%
49	14.515	2110	2113	2116	rBV2	129262	110130	1.08%	0.135%
50	14.804	2159	2162	2168	rBV3	128070	217629	2.13%	0.266%
51	15.080	2205	2209	2212	rBV	335592	485765	4.75%	0.594%
52	15.168	2221	2224	2226	rBV	142557	148252	1.45%	0.181%
53	15.386	2257	2261	2267	rVB	211432	254823	2.49%	0.311%
54	15.451	2268	2272	2278	rBV	283304	316065	3.09%	0.386%
55	15.515	2278	2283	2287	rBV	1271537	1537766	15.03%	1.879%
56	16.003	2362	2366	2370	rBV2	80588	119008	1.16%	0.145%
57	16.986	2528	2533	2541	rVB2	108706	222633	2.18%	0.272%
58	17.427	2604	2608	2620	rVB	103800	219002	2.14%	0.268%

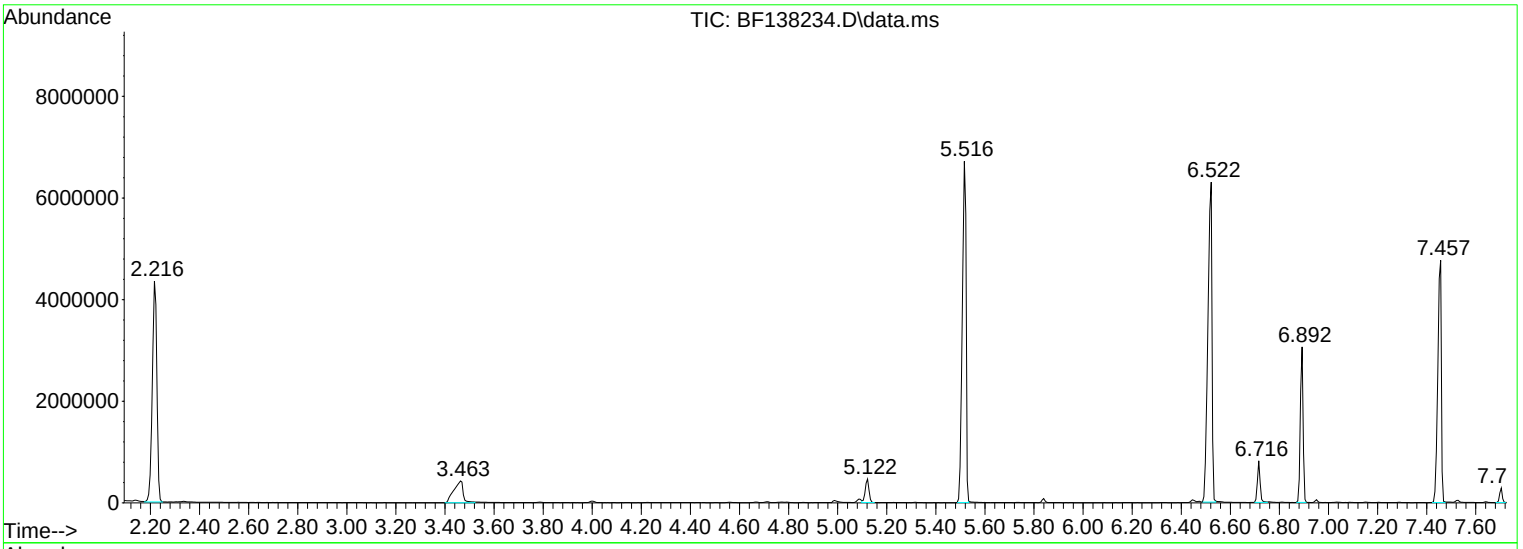
Sum of corrected areas: 81832257

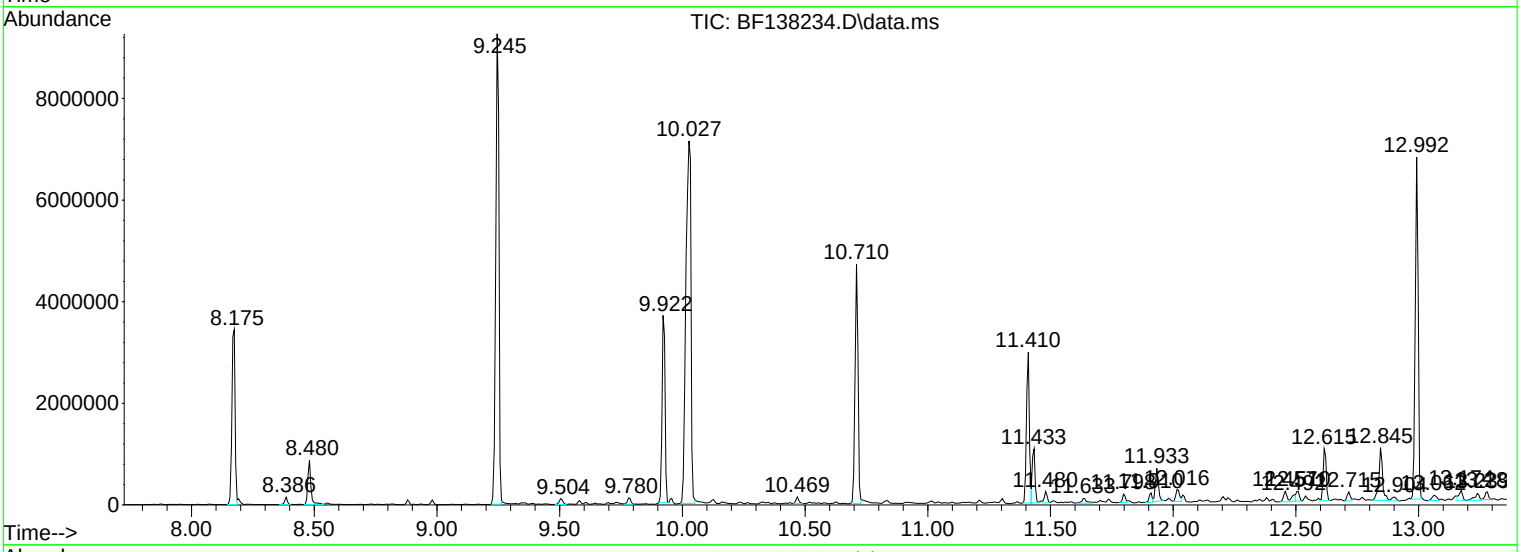
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

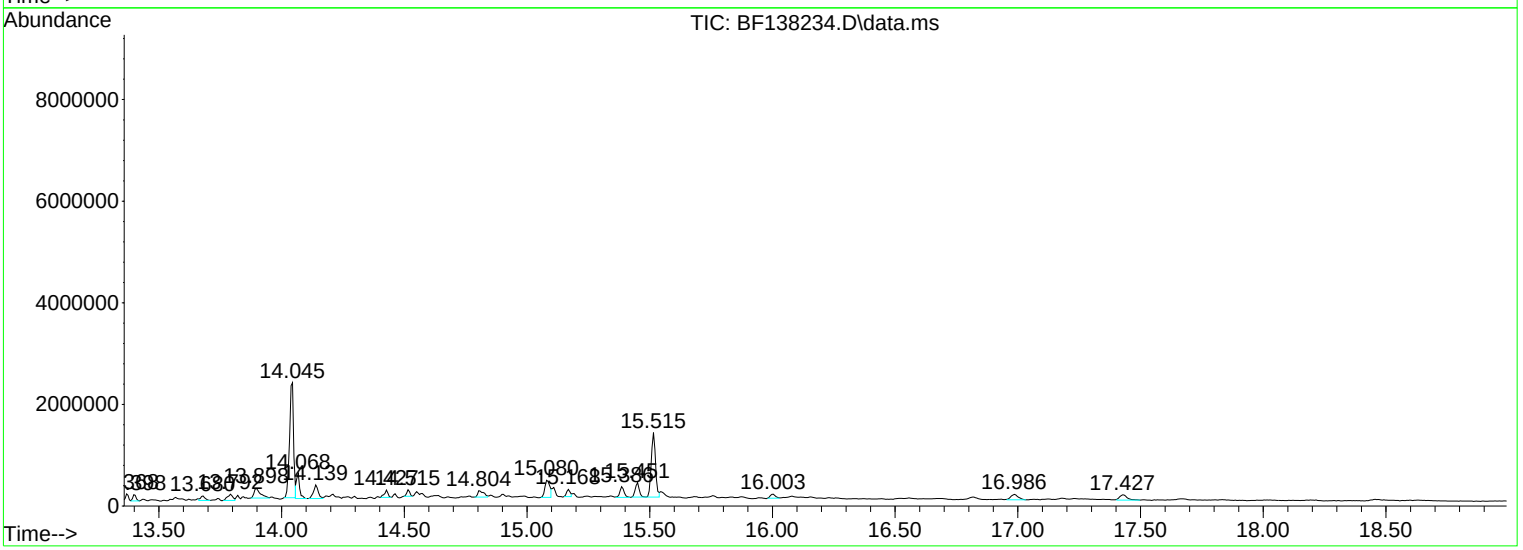
Instrument :
BNA_F
ClientSampleId :
ROAD

Quant Title :

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

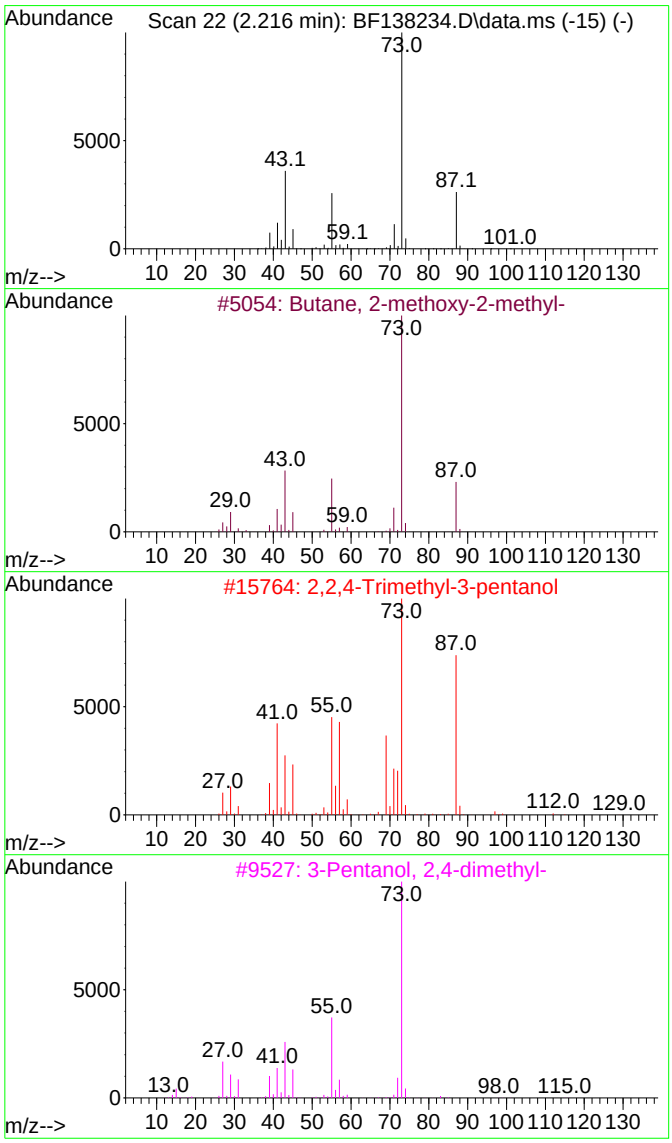
Quant Title :

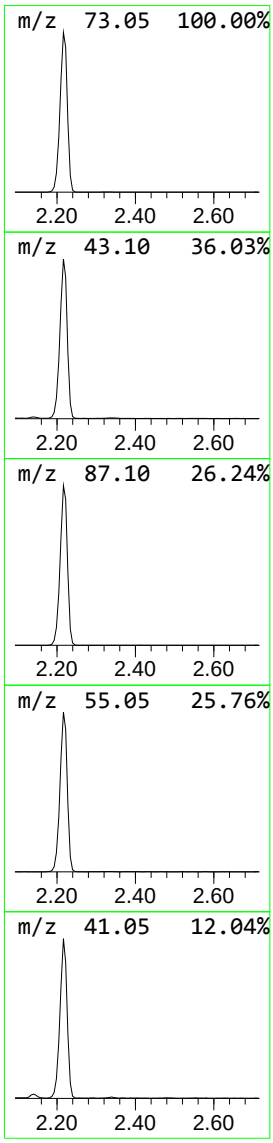
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	46.85 ng	5606540	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

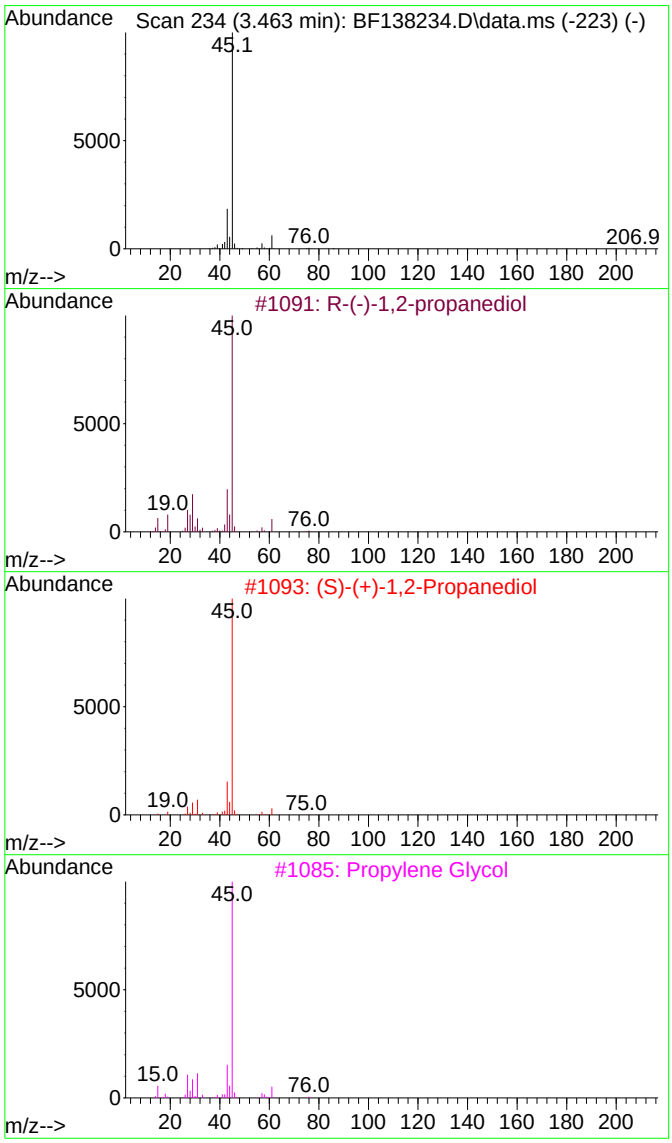
Quant Title :

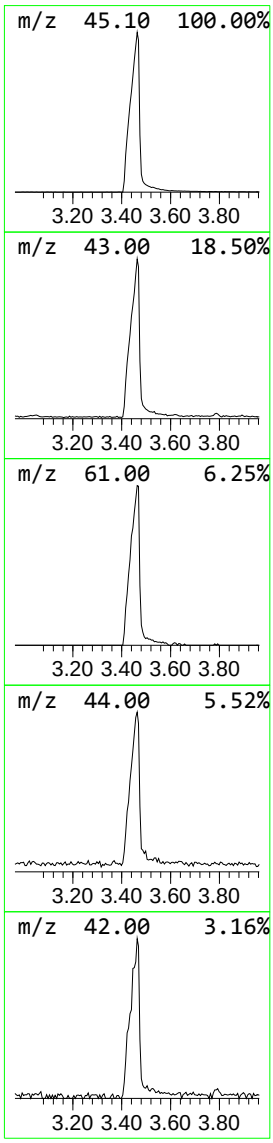
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.463	9.48 ng	1134290	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	64
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

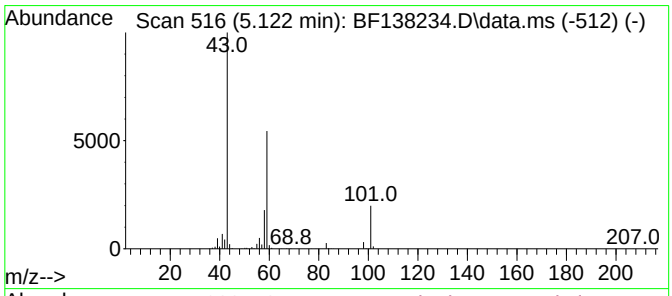
Quant Title :

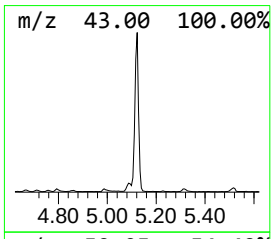
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

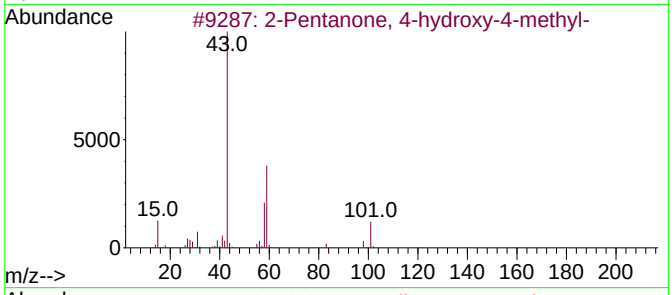
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

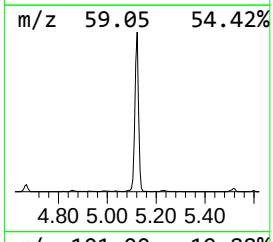
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	4.06 ng	486418	1,4-Dichlorobenzene-d4	6.892

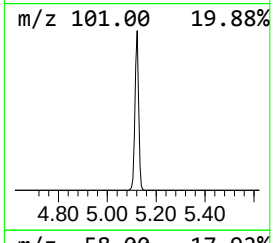
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	9

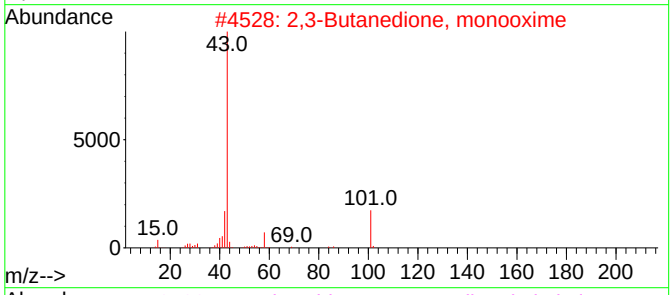


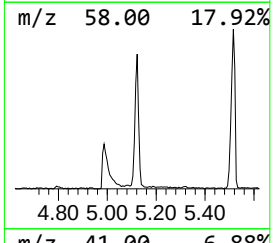


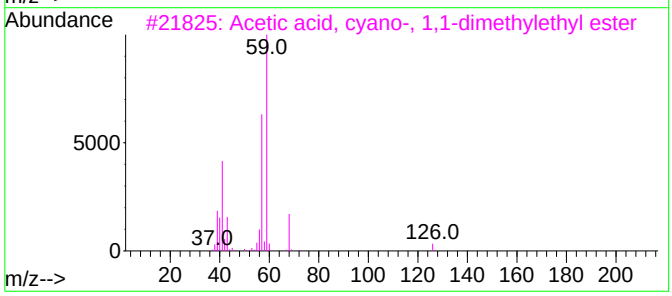


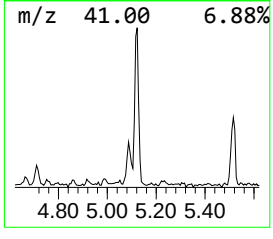












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

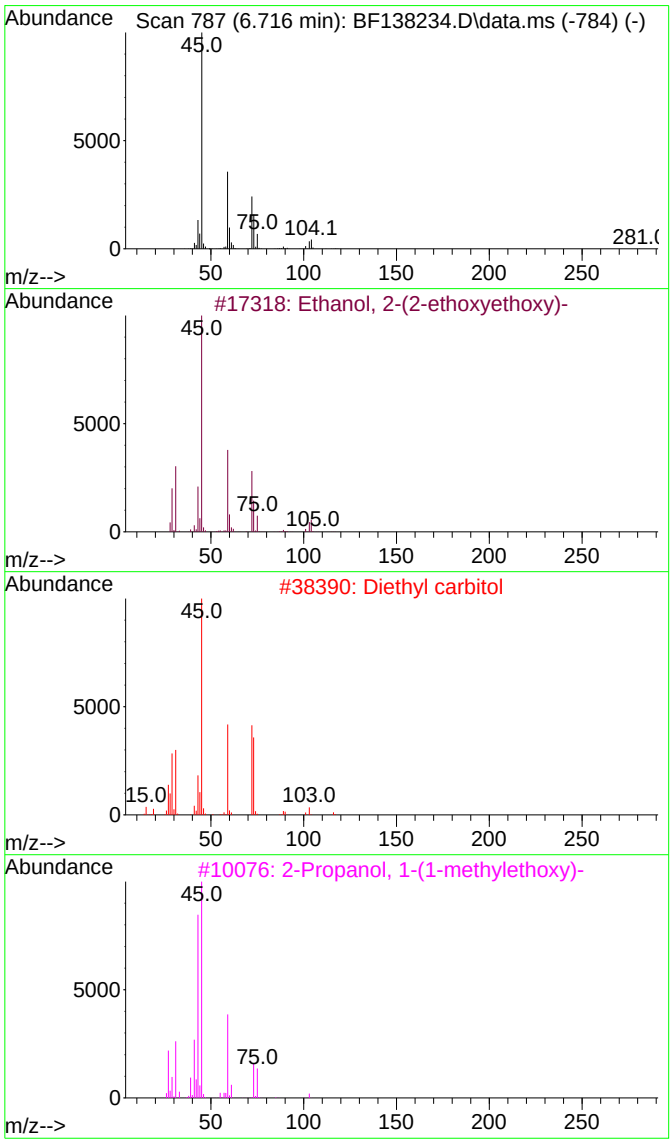
Quant Title :

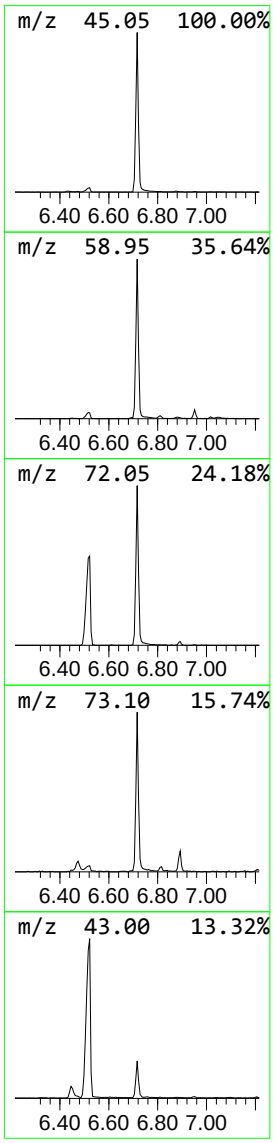
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	5.21 ng	623488	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

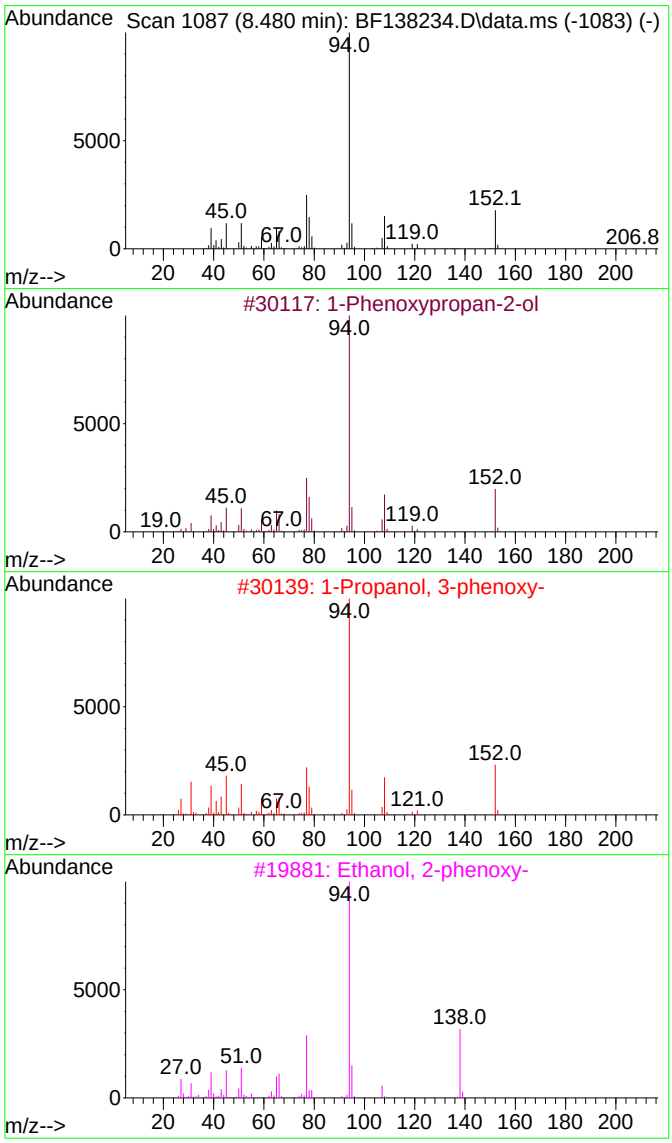
Quant Title :

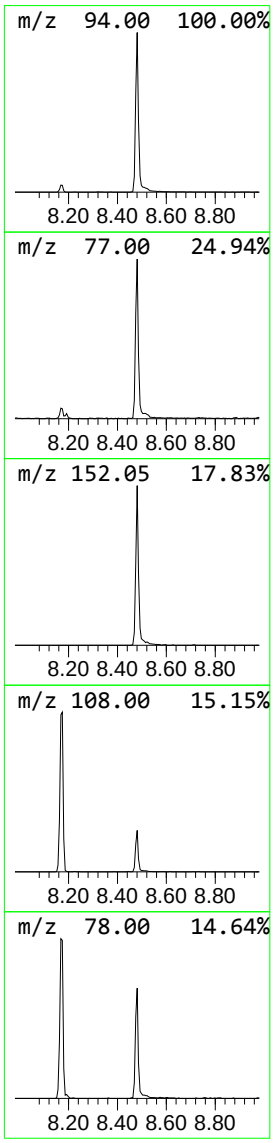
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.480	4.93 ng	771203	Naphthalene-d8	8.175

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	90
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

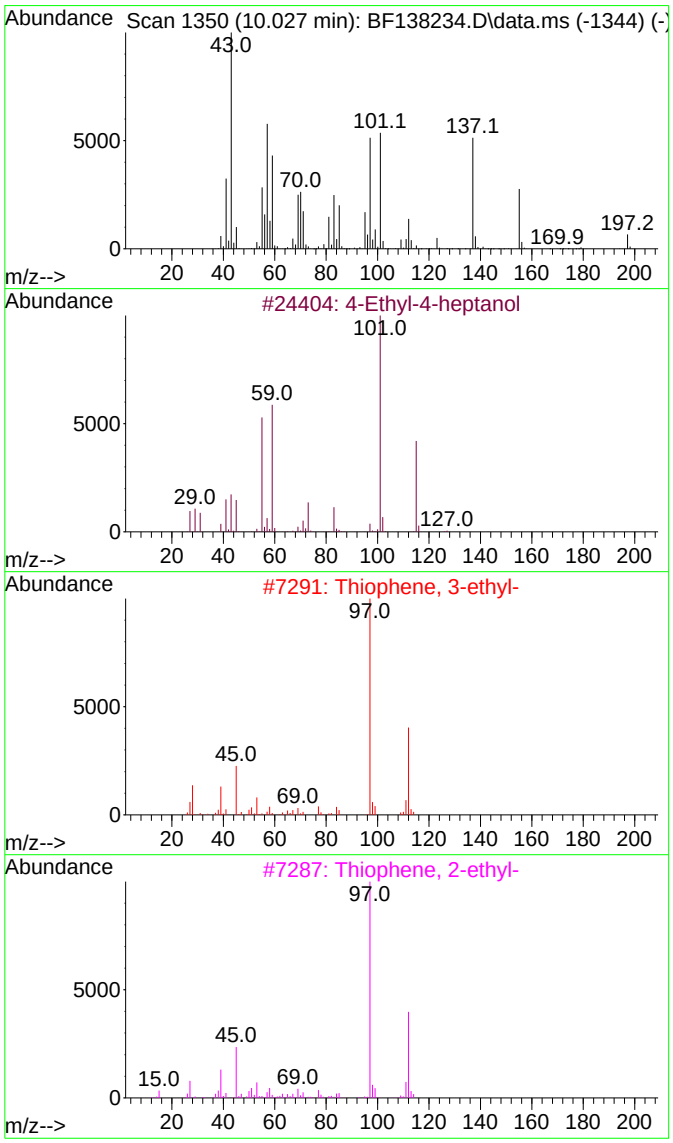
Quant Title :

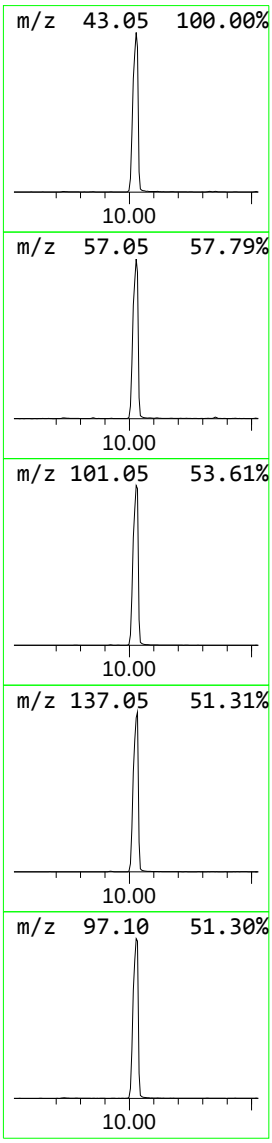
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown10.027 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.027	65.49 ng	10233500	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Ethyl-4-heptanol	144	C9H20O	000597-90-0	22
2	Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	11
3	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	11
4	Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	11
5	Acetaldehyde, 2-butenylhydrazone	112	C6H12N2	075268-07-4	11





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Data File : BF138234.D
Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

Quant Title :

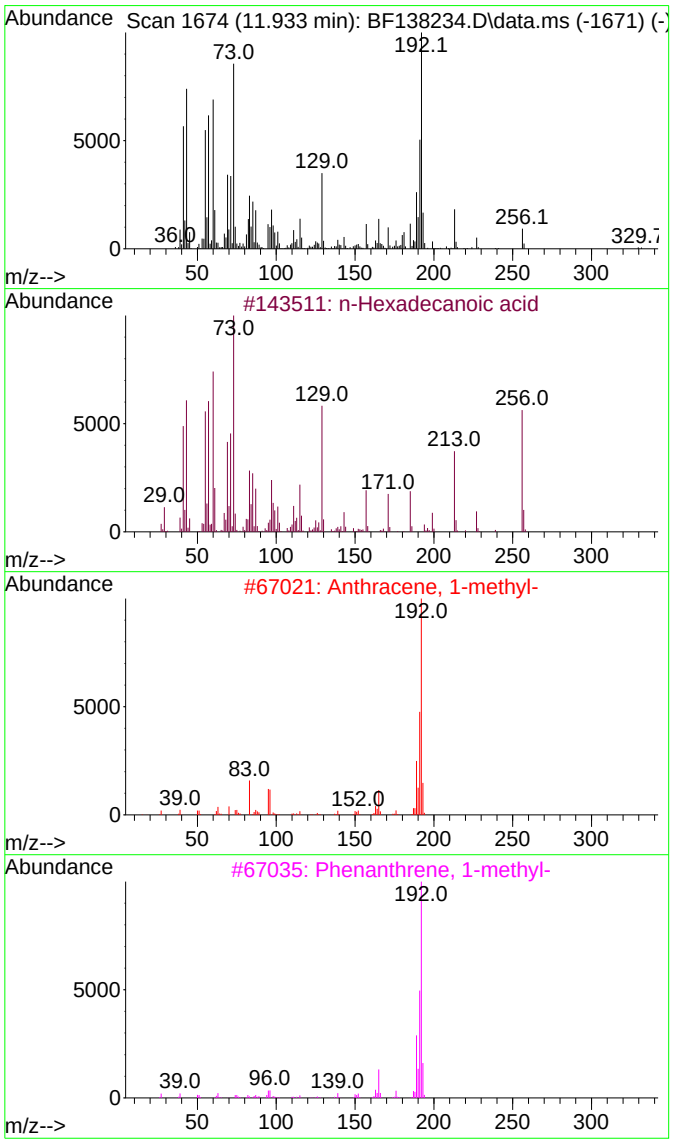
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

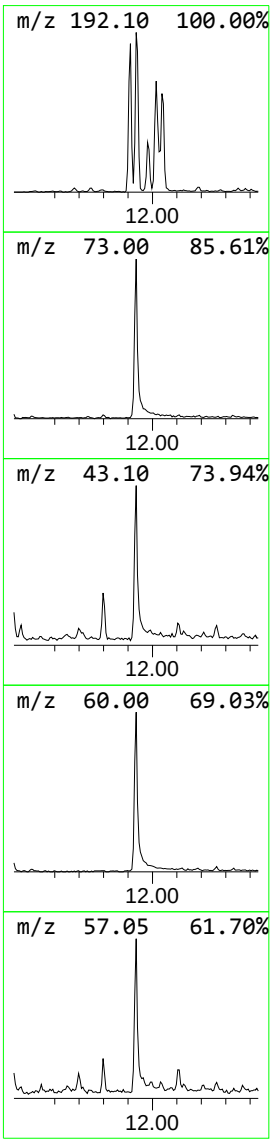
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.51 ng	562276	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94





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Acq On : 18 Jun 2024 19:59
Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROAD

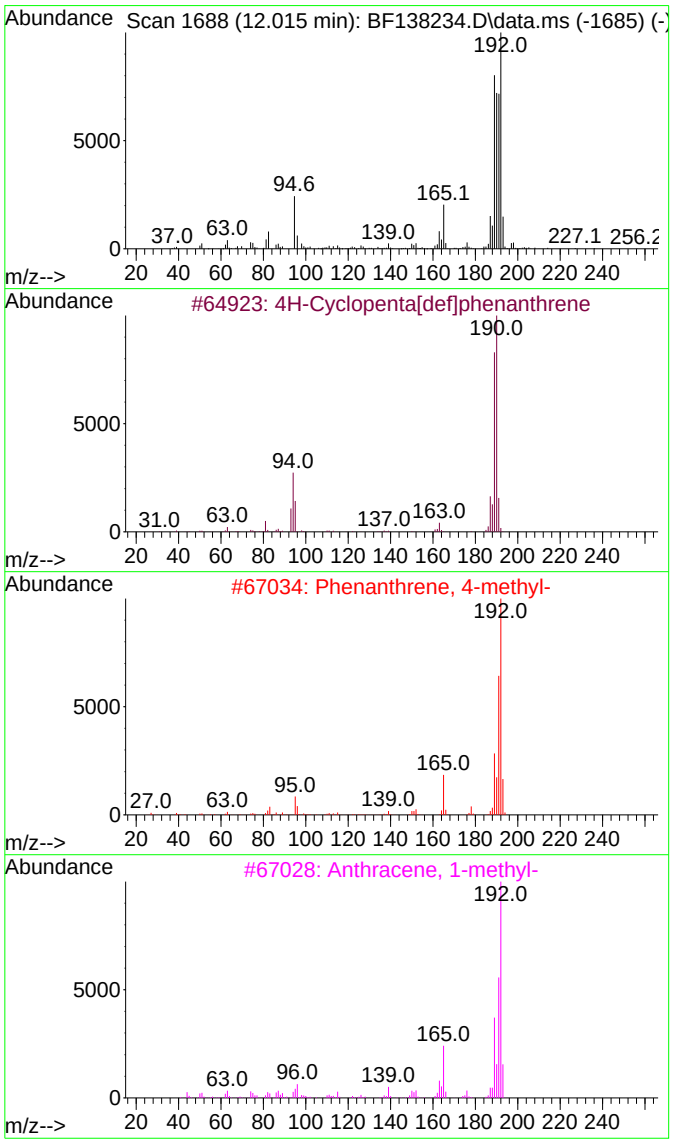
Quant Title :

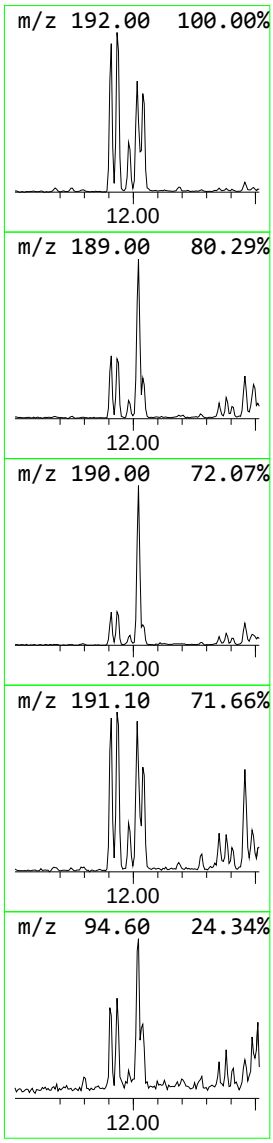
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.015	2.10 ng	262415	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	50
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	50
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	50
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	50





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Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

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Quant Title :

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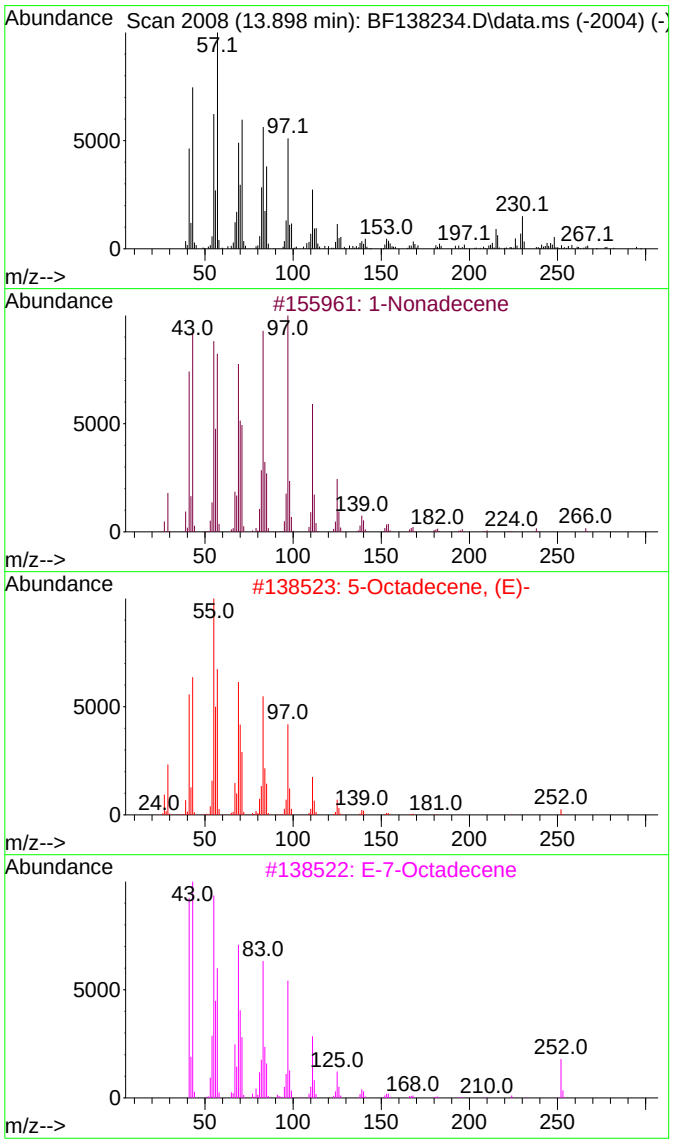
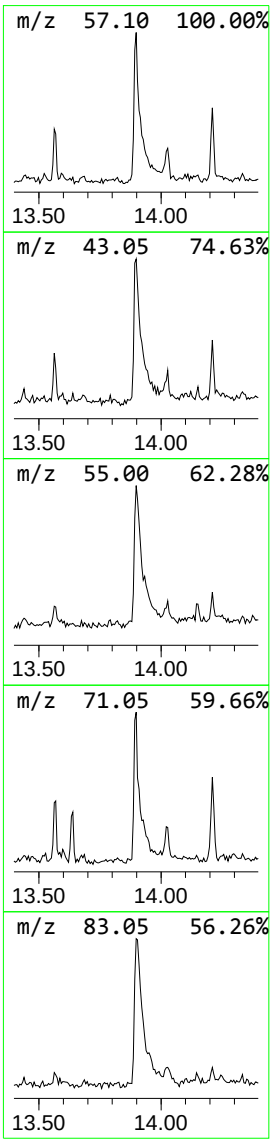
****
Peak Number 9 1-Nonadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.74 ng	354820	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	96
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
3	E-7-Octadecene	252	C18H36	1000130-92-0	90
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87





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Operator : CG\JU
Sample : P2917-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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Quant Title :

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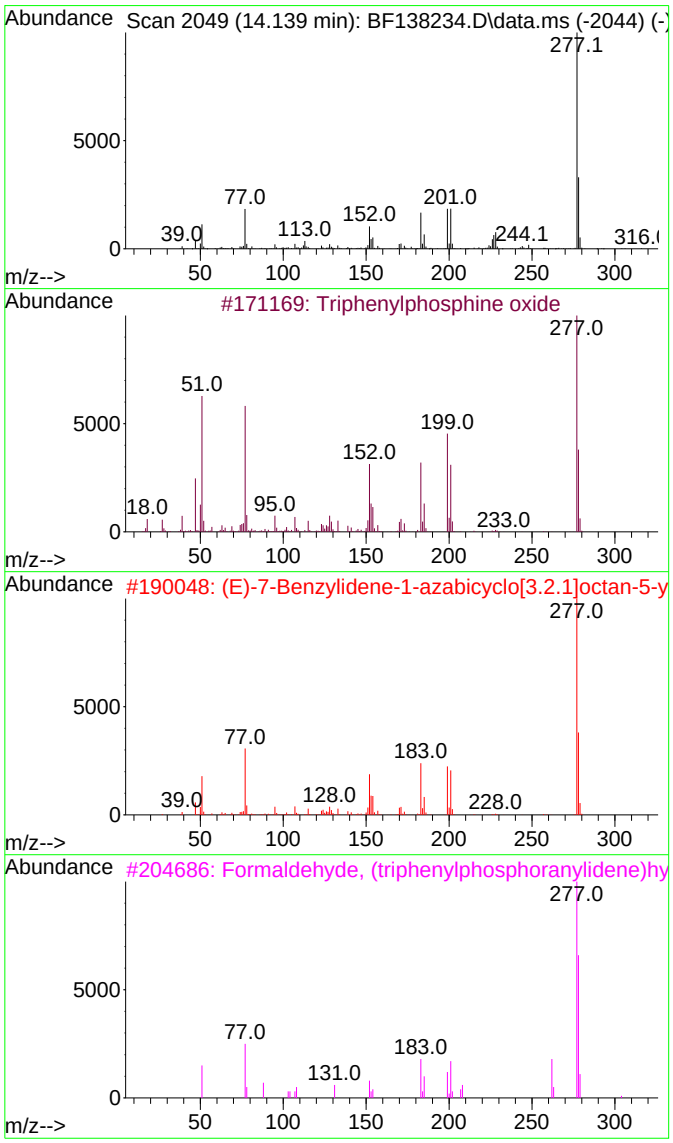
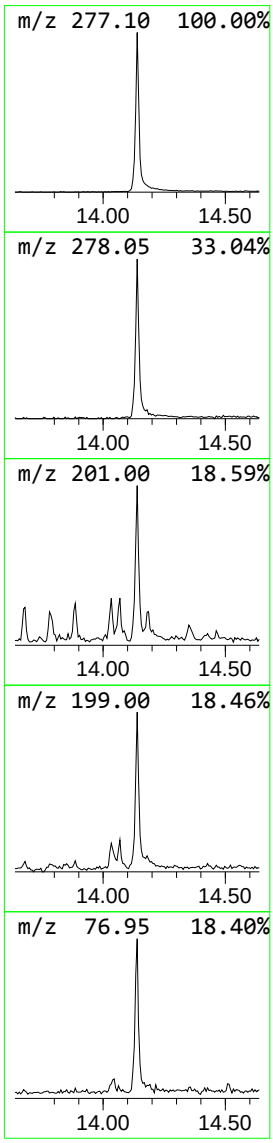
****
Peak Number 10 Triphenylphosphine oxide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	2.77 ng	359367	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	39
4	Cyclotetrasilazane, 2,2,4,4,6,6,...	292	C8H28N4Si4	001020-84-4	33
5	Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	33





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Misc :
ALS Vial : 18 Sample Multiplier: 1

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Quant Title :

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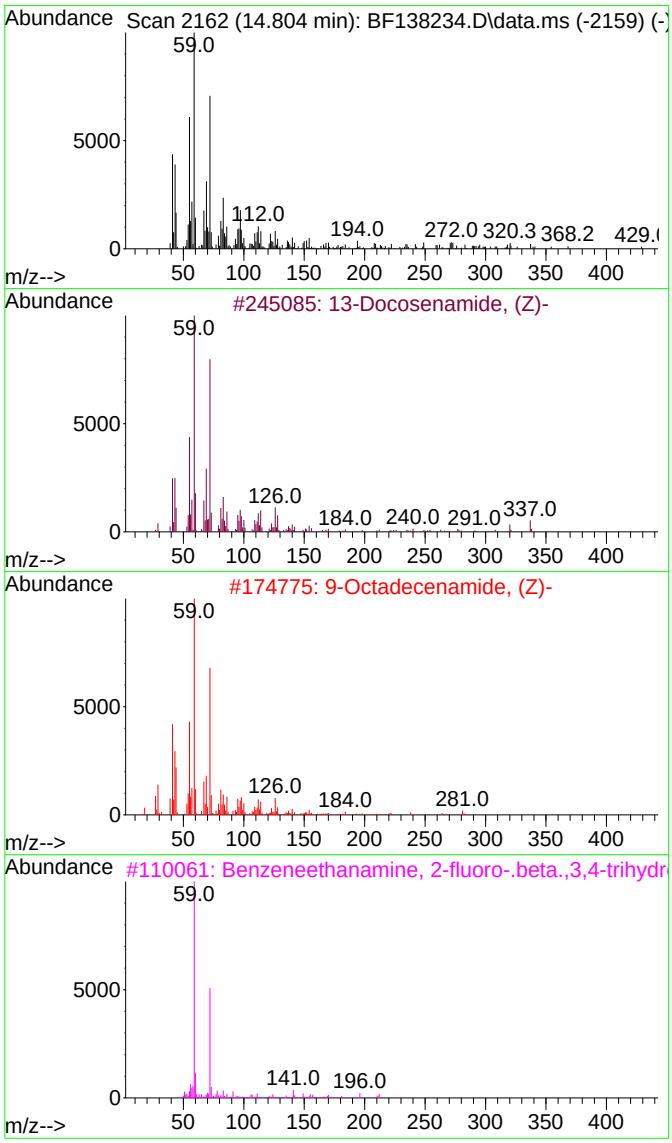
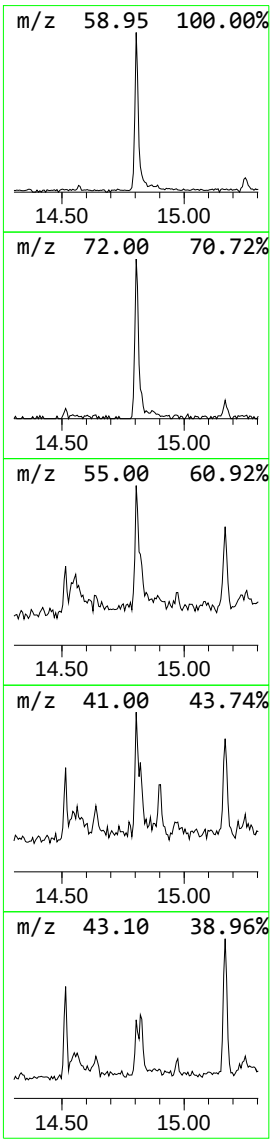
****
Peak Number 11 13-Docosenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.83 ng	217629	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
4	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	52
5	d-Glucosamine	179	C6H13NO5	000090-77-7	47





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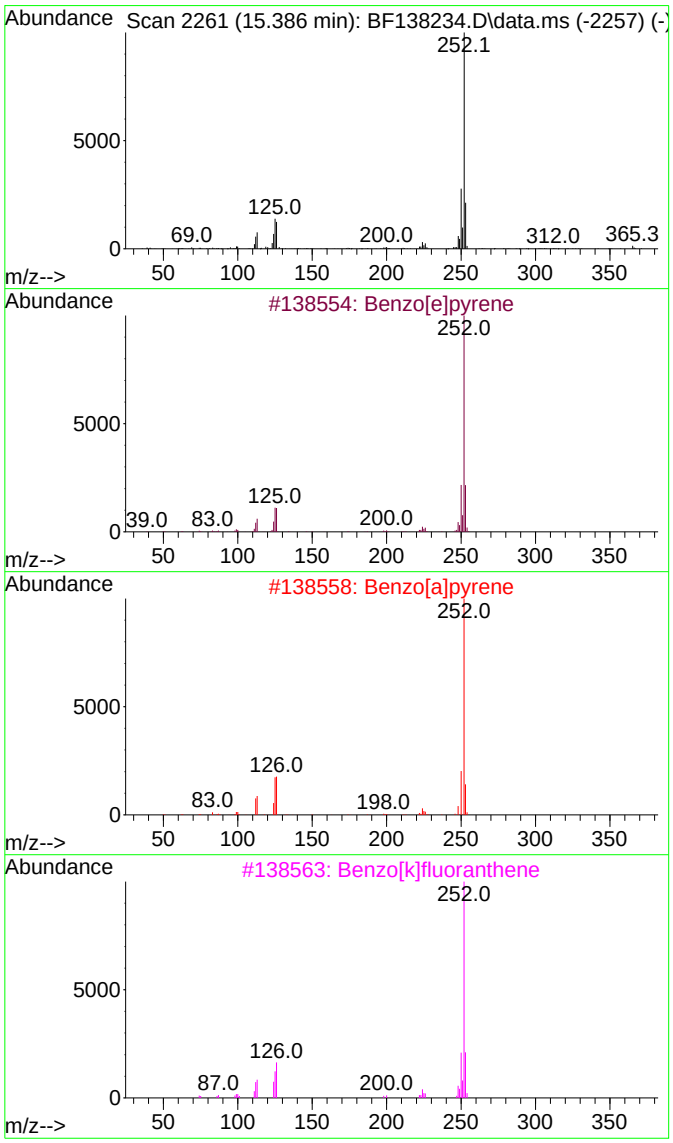
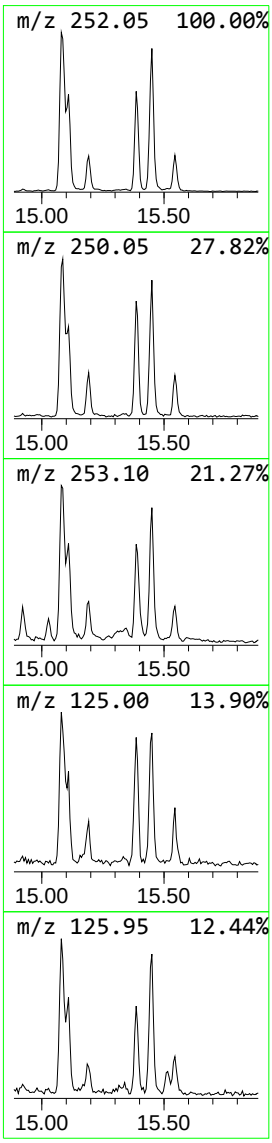
****

Peak Number 12 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	3.31 ng	254823	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	89





Tentatively Identified Compound (LSC) summary

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Data File : BF138234.D
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Instrument :
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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	Internal Standard RT	Internal Standard Resp	Internal Standard Conc
Butane, 2-metho...	2.216	46.9	ng	5606540	1	6.892	2393330	20.0
R-(-)-1,2-propa...	3.463	9.5	ng	1134290	1	6.892	2393330	20.0
2-Pentanone, 4-...	5.122	4.1	ng	486418	1	6.892	2393330	20.0
Ethanol, 2-(2-e...	6.716	5.2	ng	623488	1	6.892	2393330	20.0
1-Phenoxypropan...	8.480	4.9	ng	771203	2	8.175	3128950	20.0
unknown10.027	10.027	65.5	ng	10233500	3	9.922	3125420	20.0
n-Hexadecanoic ...	11.933	4.5	ng	562276	4	11.410	2494300	20.0
4H-Cyclopenta[d...	12.015	2.1	ng	262415	4	11.410	2494300	20.0
1-Nonadecene	13.898	2.7	ng	354820	5	14.045	2592540	20.0
Triphenylphosph...	14.139	2.8	ng	359367	5	14.045	2592540	20.0
13-Docosenamide...	14.804	2.8	ng	217629	6	15.515	1537770	20.0
Benzo[e]pyrene	15.386	3.3	ng	254823	6	15.515	1537770	20.0