LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133881.D
Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133881.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	4	9	16	rVB	451850	560785	31.47%	2.904%
2	2.252	23	28	37	rBV3	22425	36700	2.06%	0.190%
3	4.481	402	407	411	rBV	25788	28705	1.61%	0.149%
4	5.093	506	511	521	rBV	753565	885606	49.70%	4.586%
5	5.493	575	579	594	rBV	1921182	1737219	97.49%	8.996%
6	5.881	641	645	651	rBV	50212	41982	2.36%	0.217%
7	6.493	745	749	752	rBV	1798547	1694043	95.07%	8.772%
8	6.857	808	811	816	rBV	778570	650391	36.50%	3.368%
9	7.422	902	907	910	rBV	1229355	1096740	61.55%	5.679%
10	8.139	1025	1029	1032	rBV	896533	723305	40.59%	3.745%
11	9.216	1208	1212	1215	rBV	2193592	1781882	100.00%	9.227%
12	9.757	1301	1304	1308	rVB	31469	25550	1.43%	0.132%
13	9.898	1324	1328	1331	rBV	698085	618626	34.72%	3.203%
14	9.928	1331	1333	1337	rVB	28392	25492	1.43%	0.132%
15	10.445	1417	1421	1427	rBV2	20686	22460	1.26%	0.116%
16	10.610	1446	1449	1457	rVB	268632	228920	12.85%	1.185%
17	10.686	1458	1462	1469	rBV	1042548	870377	48.85%	4.507%
18	10.922	1499	1502	1506	rBV	66440	53801	3.02%	0.279%
19	11.004	1510	1516	1518	rBV	39202	43879	2.46%	0.227%
20	11.251	1553	1558	1561	rBV4	18005	23620	1.33%	0.122%
21	11.298	1565	1566	1570	rVB	29314	21873	1.23%	0.113%
22	11.386	1578	1581	1584	rBV	662901	630235	35.37%	3.263%
23	11.410	1584	1585	1589	rVV	250761	196725	11.04%	1.019%
24	11.463	1592	1594	1597	rVB	69372	54287	3.05%	0.281%
25	11.622	1617	1621	1627	rBV2	29375	38737	2.17%	0.201%
26	11.892	1662	1667	1669	rBV	47579	46960	2.64%	0.243%
27	11.922	1669	1672	1676	rVV2	129815	135074	7.58%	0.699%
28	12.004	1683	1686	1689	rBV	74661	80536	4.52%	0.417%
29	12.192	1715	1718	1720	rBV	30369	25420	1.43%	0.132%
30	12.216	1720	1722	1726	rVB2	34969	30149	1.69%	0.156%
31	12.445	1758	1761	1764	rBV	34707	40095	2.25%	0.208%
32	12.486	1765	1768	1770	rVV3	28162	29635	1.66%	0.153%
33	12.533	1773	1776	1781	rVB	38516	41571	2.33%	0.215%
34	12.610	1785	1789	1793	rBV	695386	569183	31.94%	2.947%
35	12.710	1803	1806	1808	rBV2	39534	41617	2.34%	0.216%
36	12.839	1822	1828	1834	rBV	604204	650455	36.50%	3.368%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133881.D
Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.886	1834	1836	1840	rVB2	33161	36948	2.07%	0.191%
38	12.986	1849	1853	1856	rBV	1940079	1599238	89.75%	8.281%
39	13.063	1861	1866	1869	rBV3	42534	71706	4.02%	0.371%
40	13.145	1877	1880	1882	rBV2	37928	44233	2.48%	0.229%
41	13.169	1882	1884	1888	rVB	85858	80332	4.51%	0.416%
42	13.216	1888	1892	1894	rBV	41606	48615	2.73%	0.252%
43	13.239	1894	1896	1898	rVB	54520	40559	2.28%	0.210%
44	13.274	1898	1902	1905	rBV2	63313	68396	3.84%	0.354%
45	13.369	1915	1918	1921	rBV	37995	34296	1.92%	0.178%
46	13.398	1921	1923	1927	rBV2	35898	37894	2.13%	0.196%
47	13.563	1949	1951	1955	rBV4	23662	24942	1.40%	0.129%
48	13.680	1968	1971	1976	rVB	56686	60618	3.40%	0.314%
49	13.792	1987	1990	1993	rBV3	48073	53086	2.98%	0.275%
50	13.821	1993	1995	1997	rVV	42020	37286	2.09%	0.193%
51	13.845	1997	1999	2004	rVV2	42218	60021	3.37%	0.311%
52	13.892	2004	2007	2017	rVB2	151225	214730	12.05%	1.112%
53	14.045	2027	2033	2036	rBV2	750276	1017869	57.12%	5.271%
54	14.074	2036	2038	2044	rVB	292555	260889	14.64%	1.351%
55	14.157	2049	2052	2054	rVB	48462	44485	2.50%	0.230%
56	14.439	2098	2100	2102	rVB	55552	41244	2.31%	0.214%
57	14.521	2112	2114	2118	rBV3	49634	57804	3.24%	0.299%
58	14.992	2191	2194	2197	rBV	63018	57426	3.22%	0.297%
59	15.110	2210	2214	2218	rBV	220829	359706	20.19%	1.863%
60	15.192	2225	2228	2231	rBV	129812	148958	8.36%	0.771%
61	15.427	2264	2268	2274	rVB	121434	156612	8.79%	0.811%
62	15.492	2275	2279	2285	rBV	158018	194872	10.94%	1.009%
63	15.557	2286	2290	2294	rBV	292907	390971	21.94%	2.025%
64	16.063	2372	2376	2382	rVB	83320	123838	6.95%	0.641%
65	17.104	2548	2553	2564	rVB2	70777	161509	9.06%	0.836%

Sum of corrected areas: 19311718

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
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Instrument :
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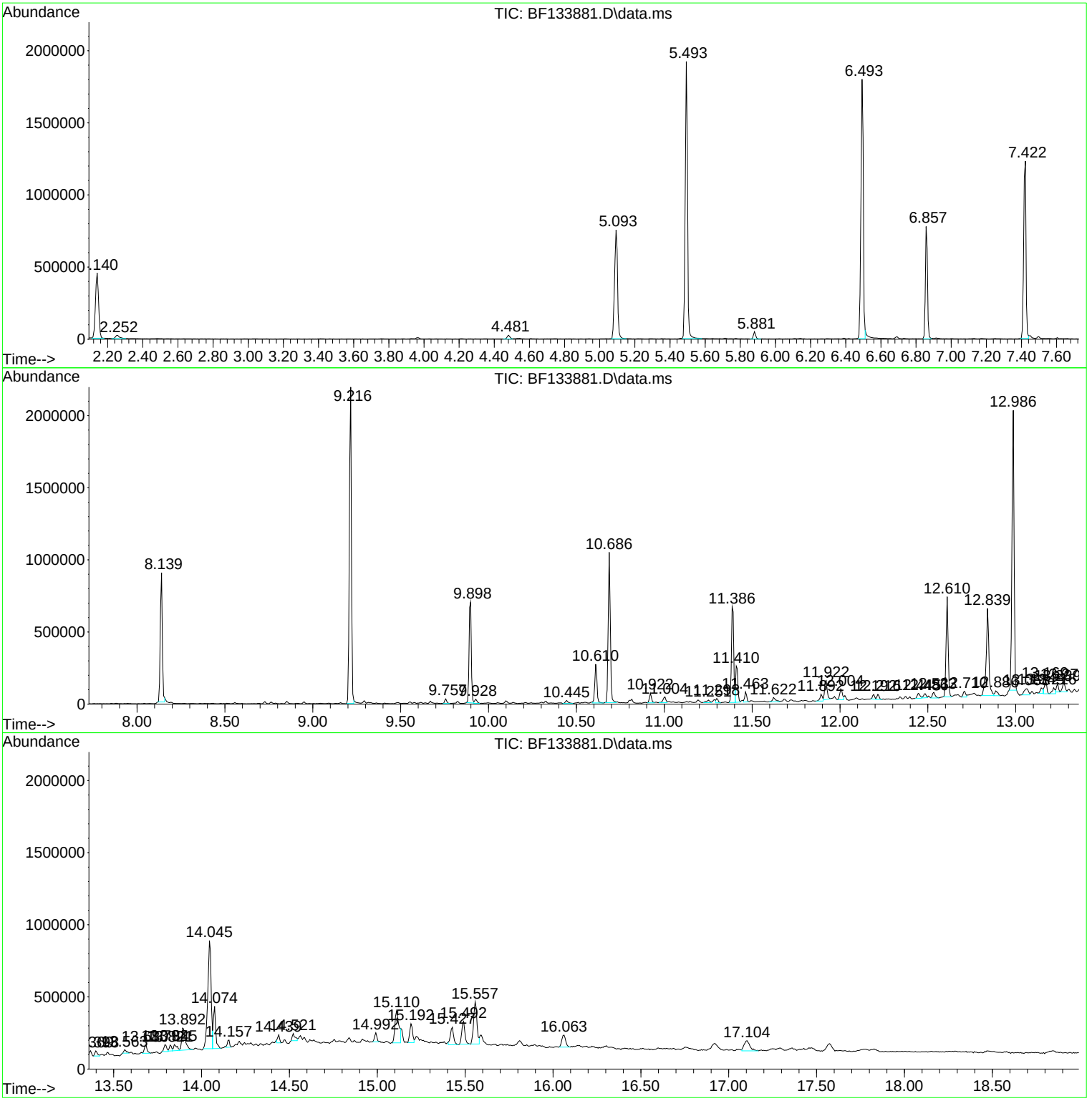
ClientSampleId :
COMPOSIT-TW-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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\BF062123\
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BNA_F
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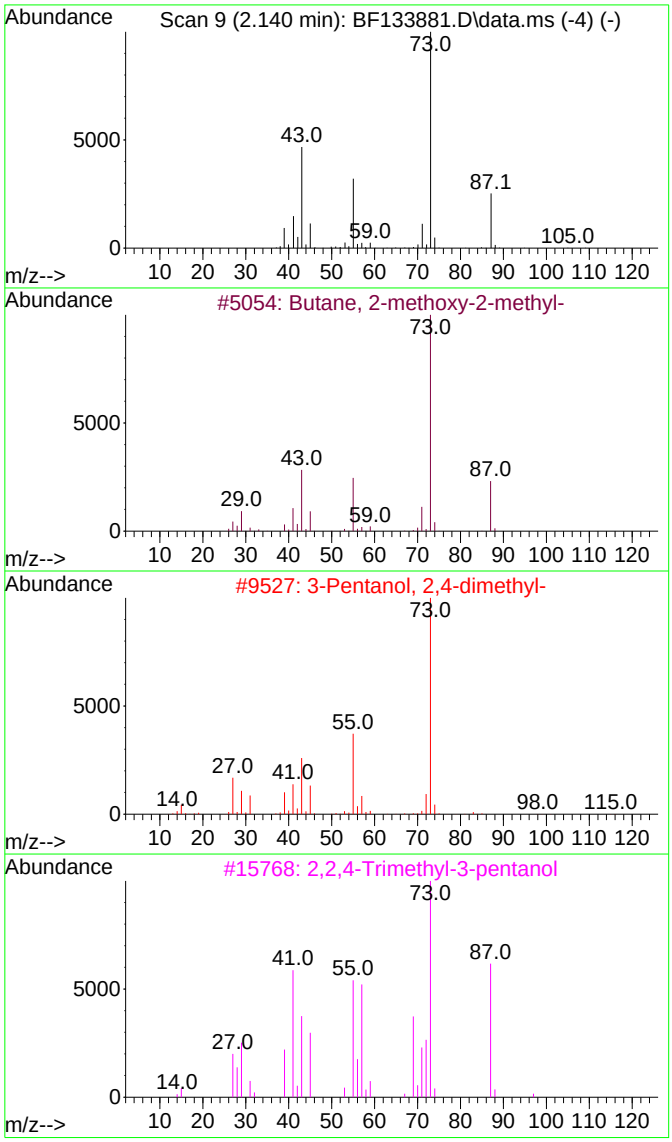
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

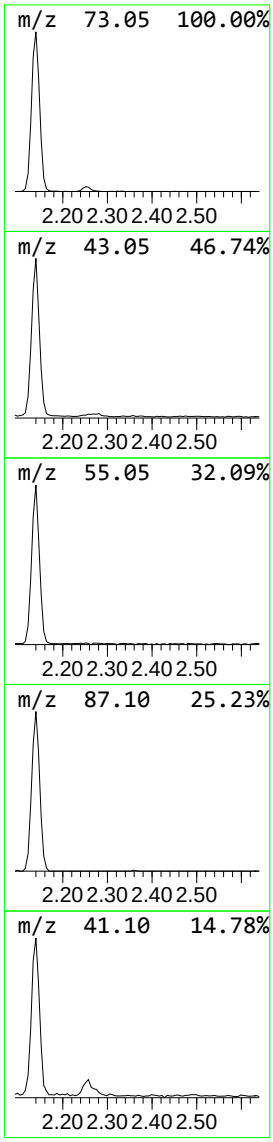
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	17.24 ng	560785	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133881.D
Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

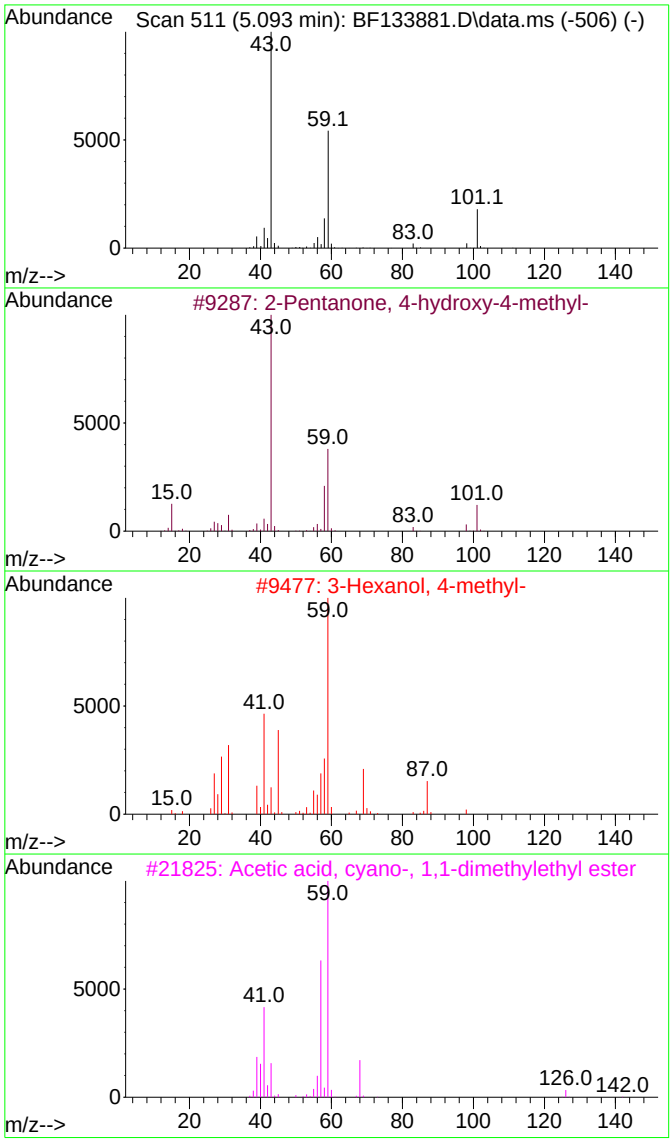
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

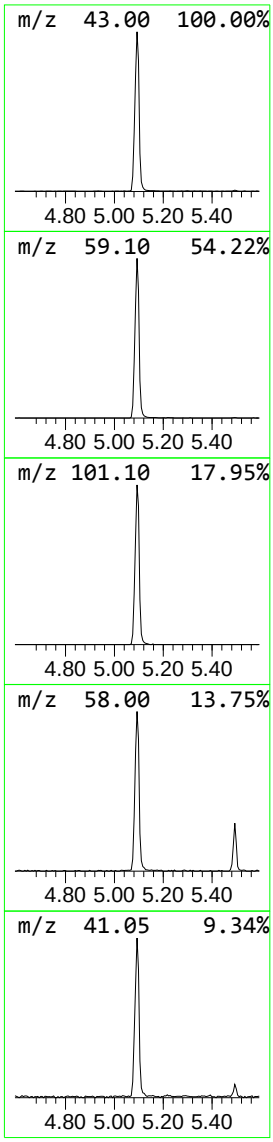
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	27.23 ng	885606	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133881.D
Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

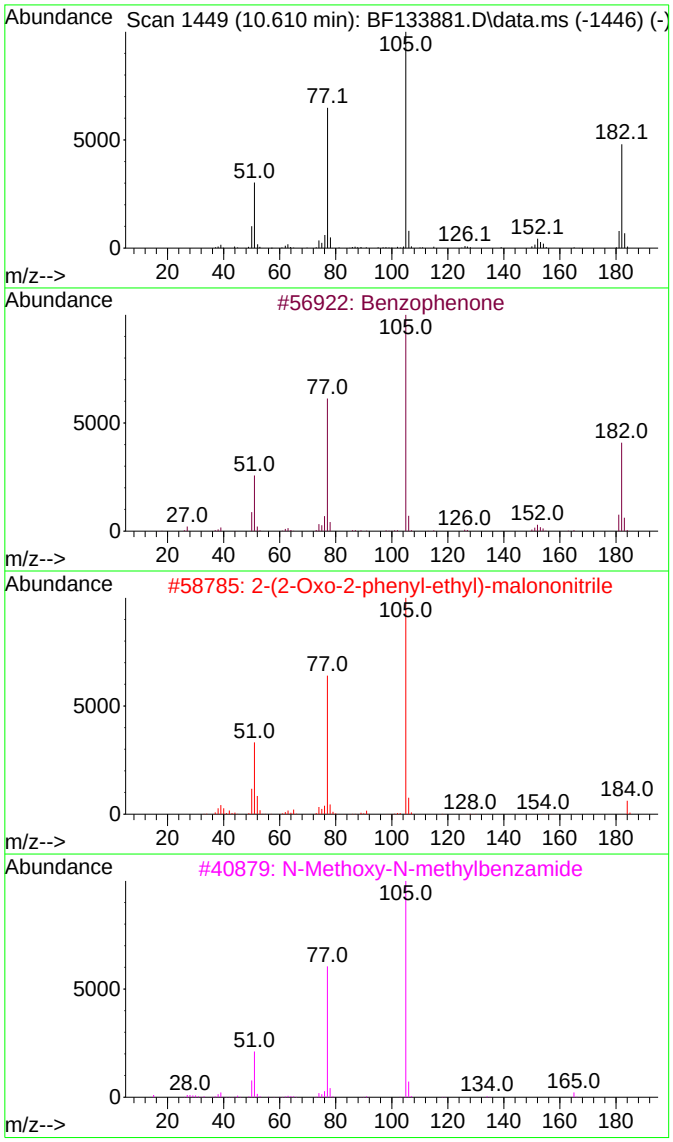
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

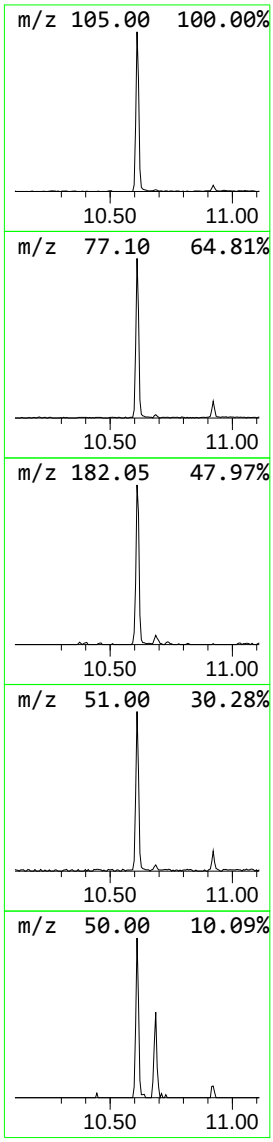
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	7.40 ng	228920	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	58
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50
5	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
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Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

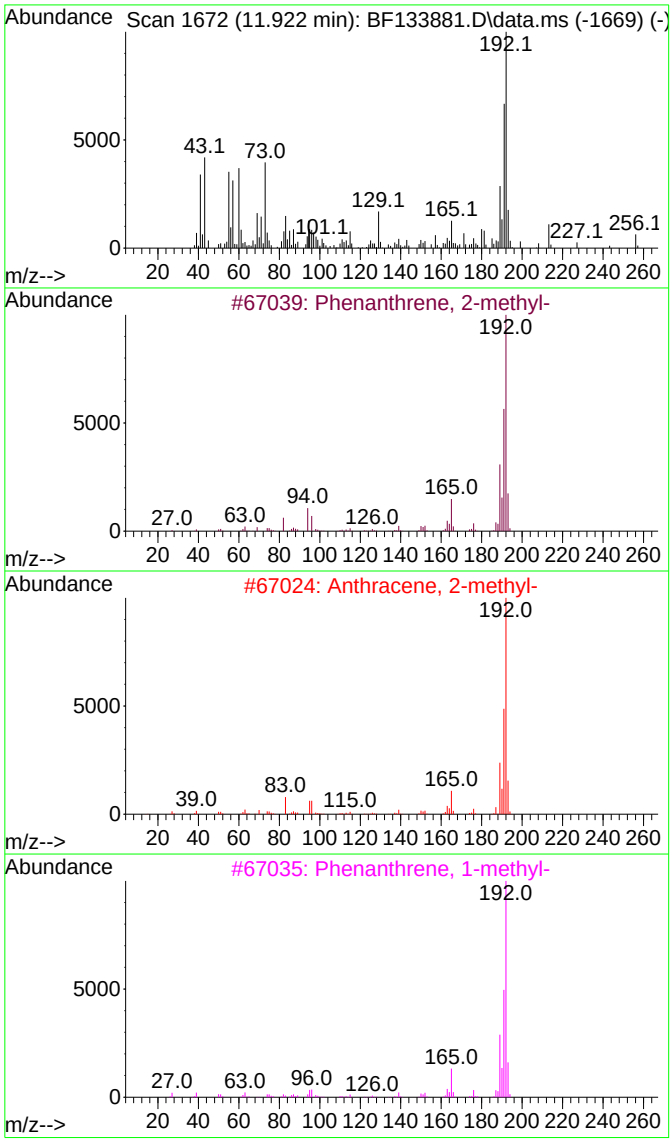
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

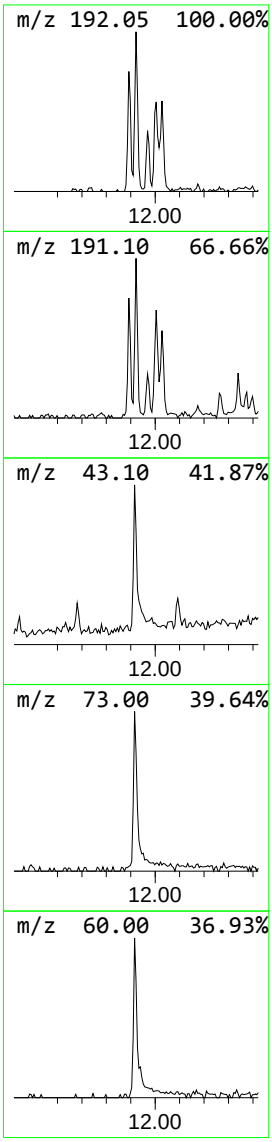
****

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	4.29 ng	135074	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133881.D
Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

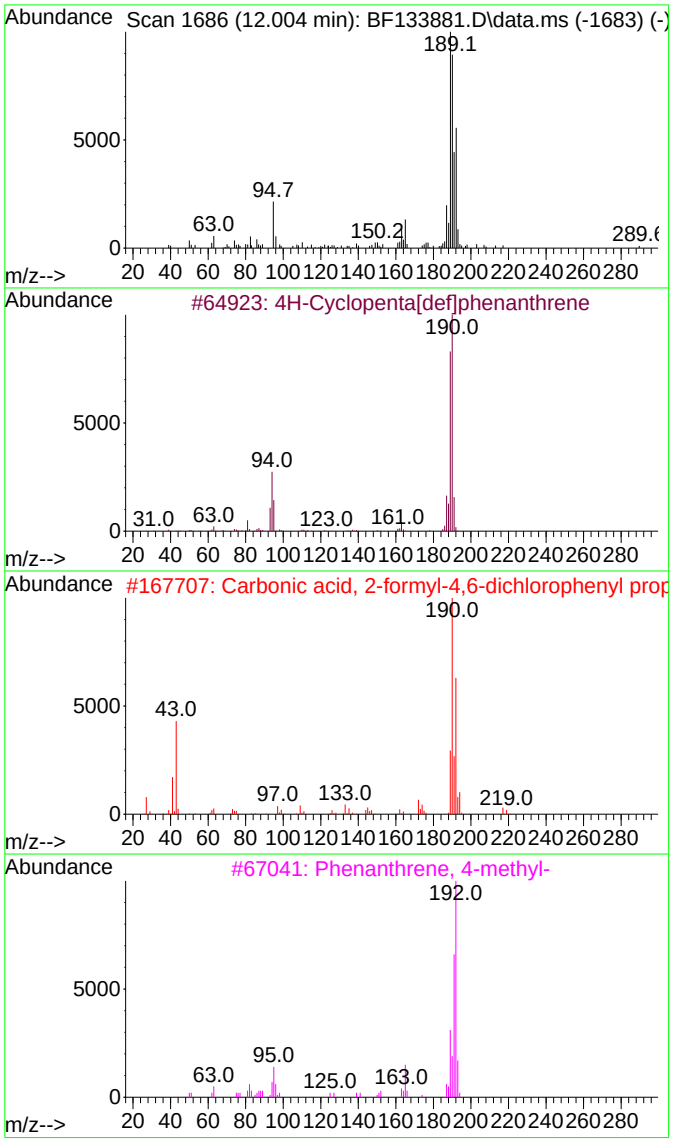
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

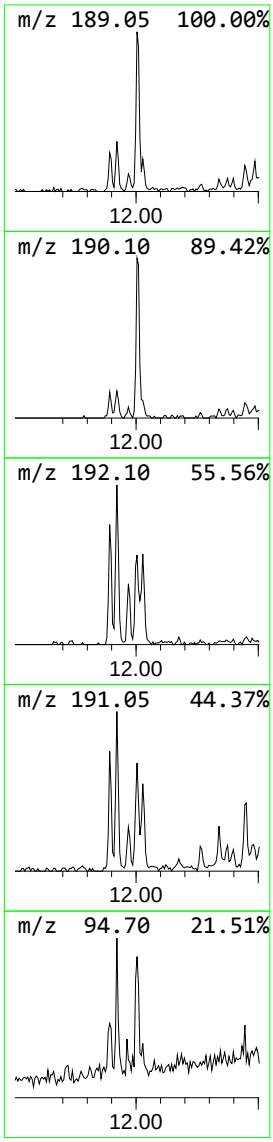
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	2.56 ng	80536	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Carbonic acid, 2-formyl-4,6-dich...	276	C11H10Cl2O4	1000331-39-3	38
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	22





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

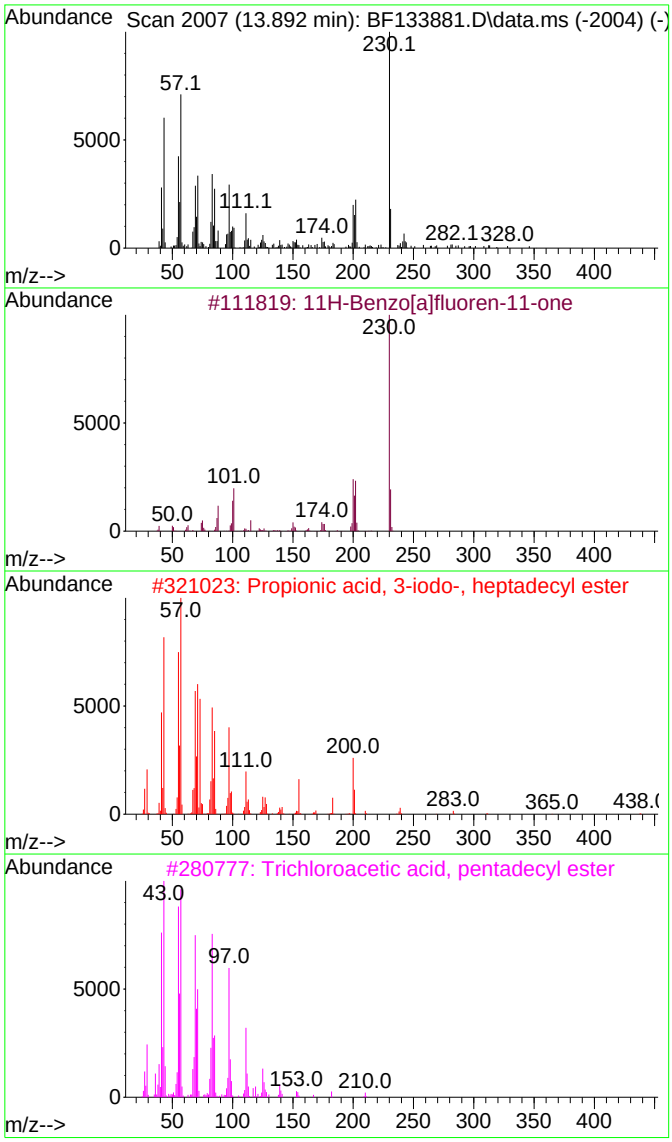
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

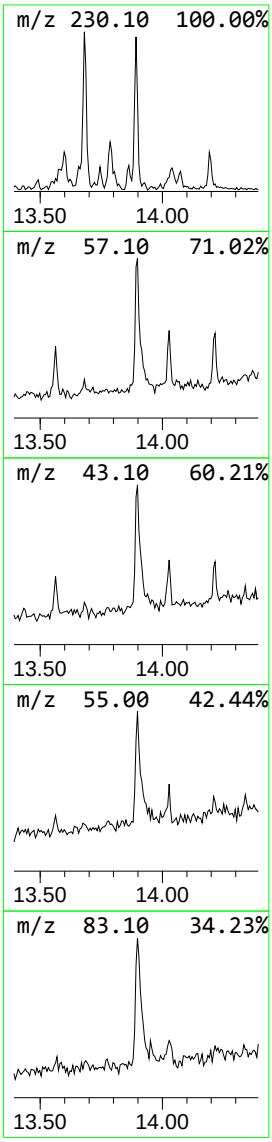
****

Peak Number 6 11H-Benzo[a]fluoren-11-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.22 ng	214730	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	89
2	Propionic acid, 3-iodo-, heptade...	438	C20H39IO2	1000406-24-8	38
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	25
4	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	25
5	Propionic acid, 3-iodo-, octadec...	452	C21H41IO2	1000406-24-9	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133881.D
Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

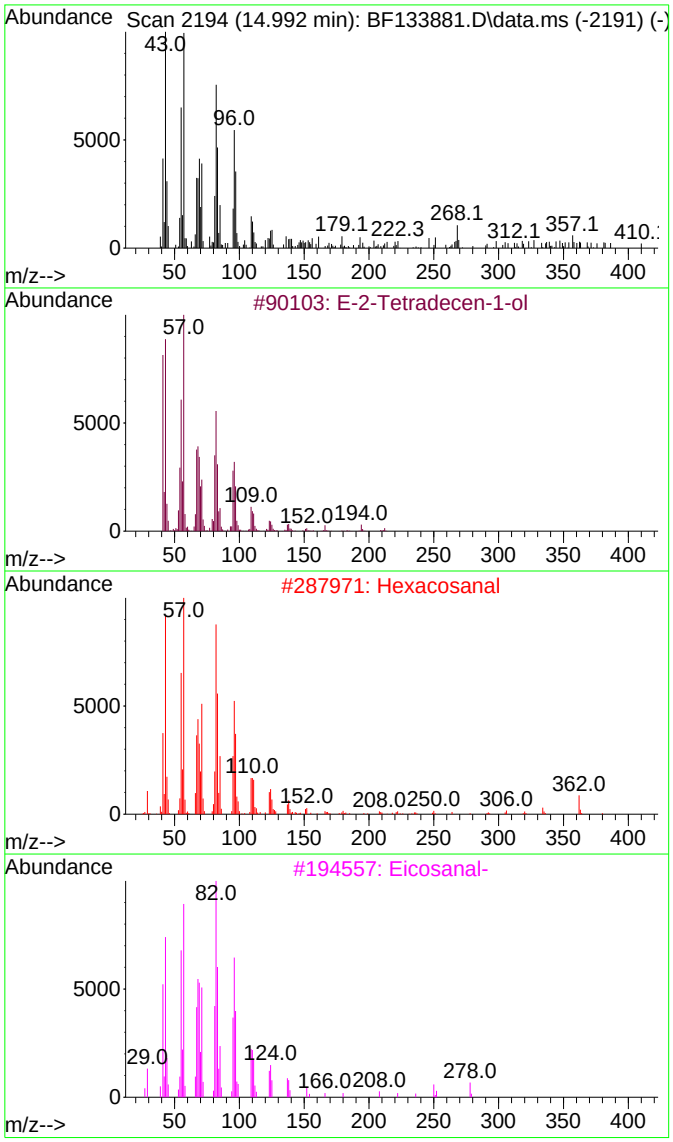
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

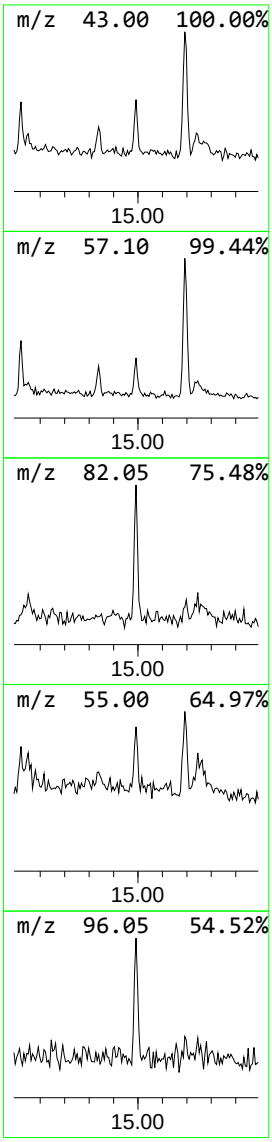
****

Peak Number 7 E-2-Tetradecen-1-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	2.94 ng	57426	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	90
2	Hexacosanal	380	C26H52O	026627-85-0	80
3	Eicosanal-	296	C20H40O	002400-66-0	64
4	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	50
5	2-Cyclohexylnonadecane	350	C25H50	1000357-24-9	46





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Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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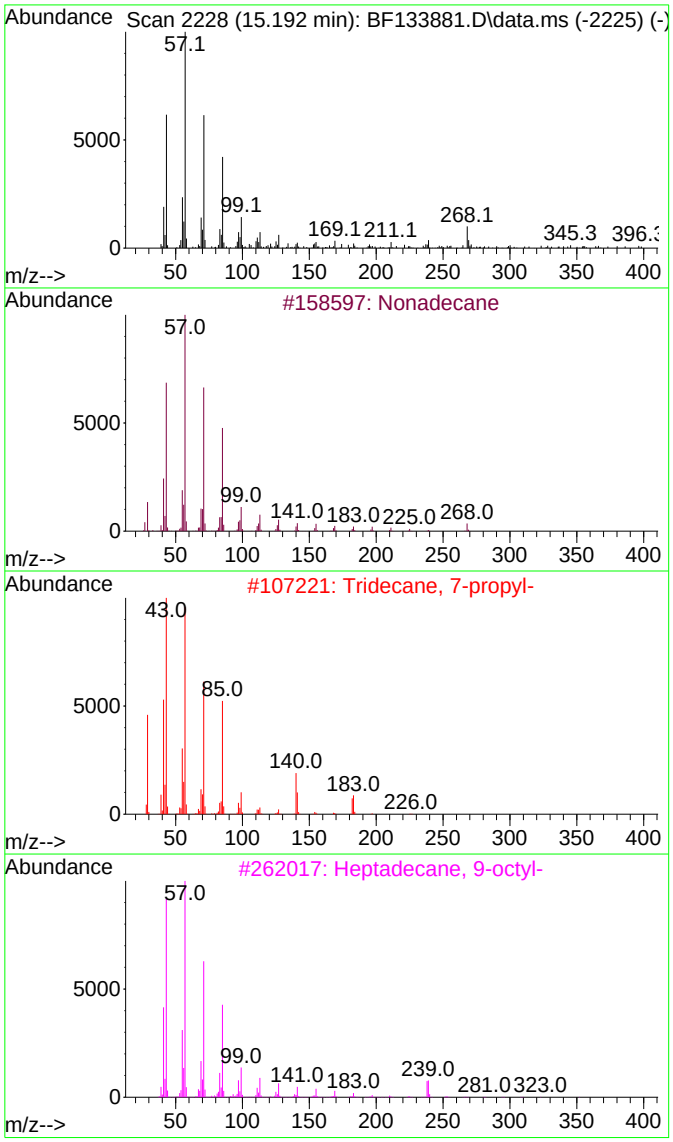
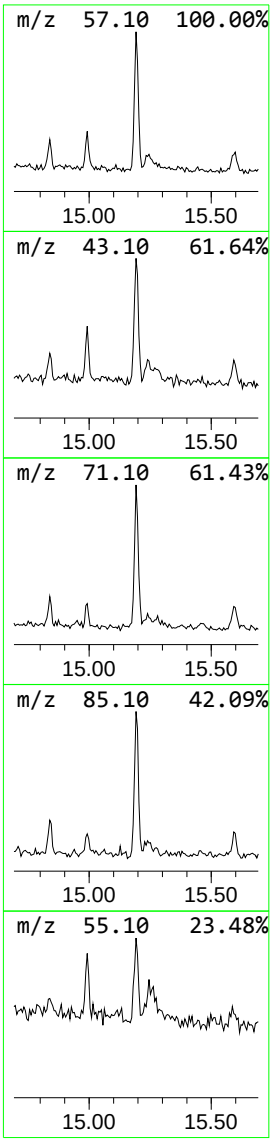
Peak Number 8 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	7.62 ng	148958	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Tridecane, 7-propyl-	226	C16H34	055045-09-5	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptacosane	380	C27H56	000593-49-7	83





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Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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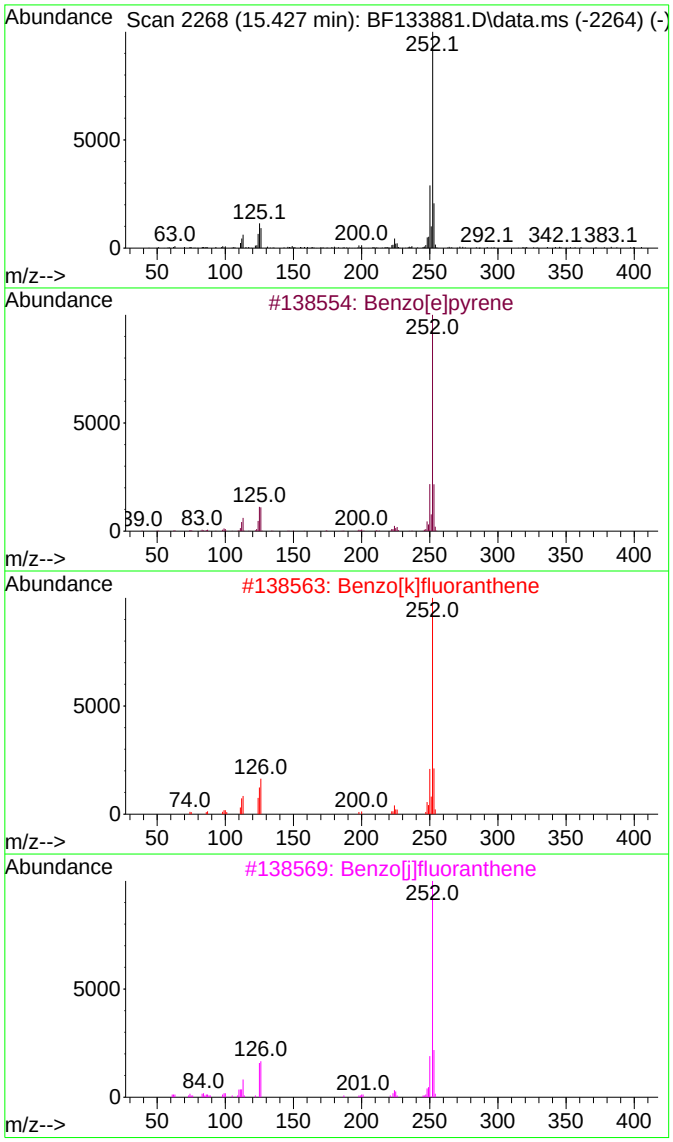
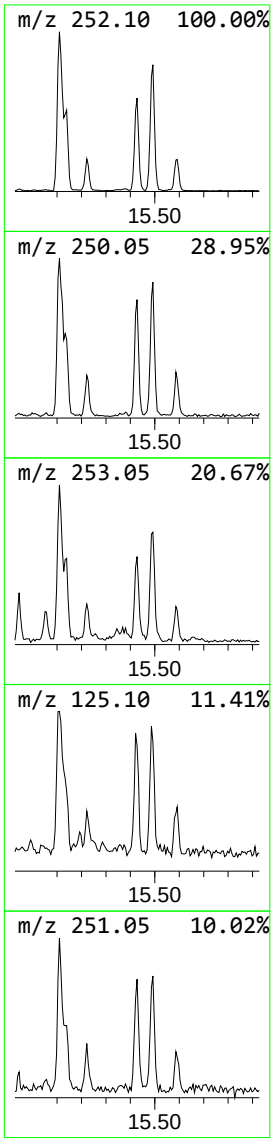
Peak Number 9 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	8.01 ng	156612	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133881.D
Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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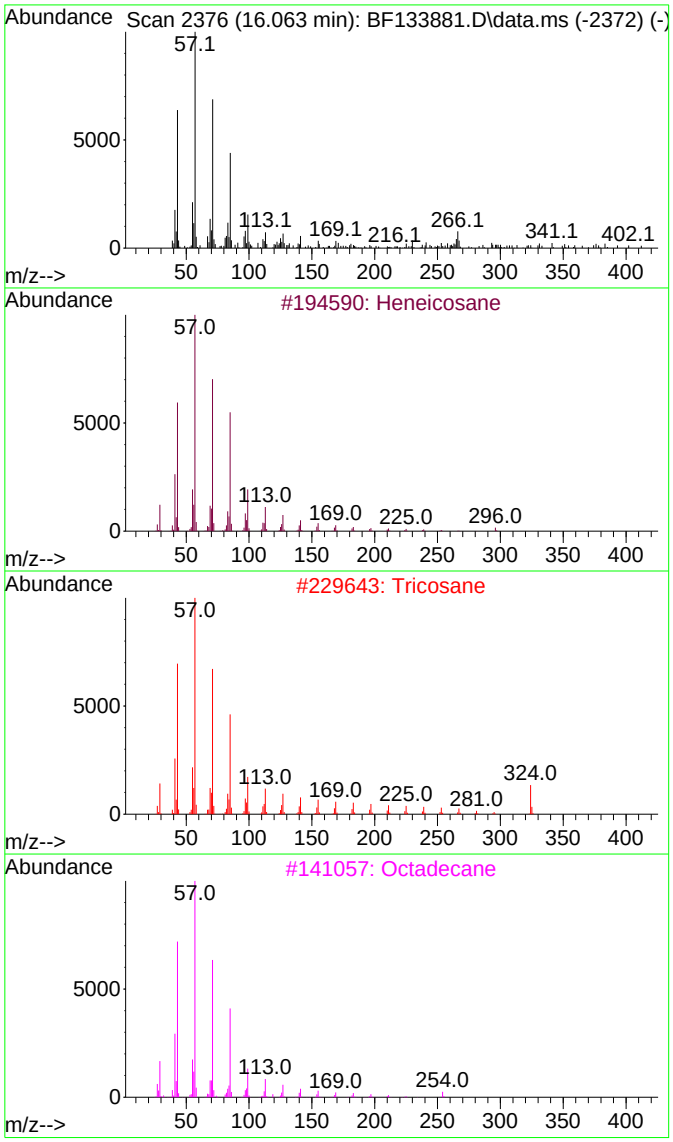
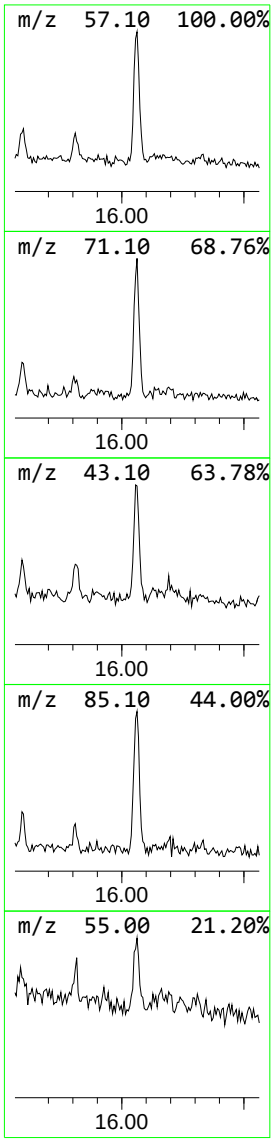
Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.063	6.33 ng	123838	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Tricosane	324	C23H48	000638-67-5	89
3	Octadecane	254	C18H38	000593-45-3	89
4	Heptadecane	240	C17H36	000629-78-7	89
5	Pentacosane	352	C25H52	000629-99-2	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133881.D
Acq On : 21 Jun 2023 20:38
Operator : CG\JU
Sample : 03298-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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
Butane, 2-metho...	2.140	17.2	ng	560785	1	6.857	650391	20.0
2-Pentanone, 4-...	5.093	27.2	ng	885606	1	6.857	650391	20.0
Benzophenone	10.610	7.4	ng	228920	3	9.898	618626	20.0
Phenanthrene, 2...	11.922	4.3	ng	135074	4	11.386	630235	20.0
4H-Cyclopenta[d...	12.004	2.6	ng	80536	4	11.386	630235	20.0
11H-Benzo[a]flu...	13.892	4.2	ng	214730	5	14.051	1017870	20.0
E-2-Tetradecen-...	14.992	2.9	ng	57426	6	15.557	390971	20.0
Nonadecane	15.192	7.6	ng	148958	6	15.557	390971	20.0
Benzo[e]pyrene	15.427	8.0	ng	156612	6	15.557	390971	20.0
Heneicosane	16.063	6.3	ng	123838	6	15.557	390971	20.0