LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102623\
Data File : BF135961.D
Acq On : 26 Oct 2023 14:00
Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

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-BF102523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	666205	723888	18.30%	2.117%
2	2.228	20	24	29	rVB	54183	66387	1.68%	0.194%
3	5.057	499	505	514	rVB	501795	613580	15.51%	1.794%
4	5.451	567	572	575	rBV	3452888	3445249	87.11%	10.076%
5	6.451	736	742	745	rBV	3410929	3481538	88.03%	10.182%
6	6.822	802	805	808	rBV	1405389	1070433	27.07%	3.131%
7	7.386	896	901	903	rBV	2308947	2151132	54.39%	6.291%
8	8.104	1019	1023	1026	rBV	1813419	1455773	36.81%	4.257%
9	8.863	1149	1152	1156	rBV	175694	134390	3.40%	0.393%
10	9.180	1202	1206	1209	rBV	4398551	3954855	100.00%	11.566%
11	9.304	1224	1227	1231	rVB	73668	67727	1.71%	0.198%
12	9.516	1257	1263	1266	rBV2	51948	67799	1.71%	0.198%
13	9.839	1313	1318	1319	rBV	129181	120439	3.05%	0.352%
14	9.857	1319	1321	1325	rVV	1819127	1619124	40.94%	4.735%
15	9.892	1325	1327	1336	rVB	220108	178209	4.51%	0.521%
16	9.986	1340	1343	1346	rVB	87550	66508	1.68%	0.195%
17	10.063	1353	1356	1360	rBV	186204	146238	3.70%	0.428%
18	10.410	1411	1415	1418	rBV	240518	211511	5.35%	0.619%
19	10.651	1451	1456	1459	rBV	2882673	2446043	61.85%	7.154%
20	10.680	1459	1461	1470	rVB	44414	60393	1.53%	0.177%
21	11.245	1553	1557	1563	rVB	50816	48817	1.23%	0.143%
22	11.351	1571	1575	1577	rBV	2020759	1664218	42.08%	4.867%
23	11.374	1577	1579	1582	rVV	638213	472734	11.95%	1.383%
24	11.422	1582	1587	1590	rVB	126350	121054	3.06%	0.354%
25	11.580	1607	1614	1617	rBV	178818	147791	3.74%	0.432%
26	11.851	1656	1660	1663	rBV	69643	63274	1.60%	0.185%
27	11.892	1663	1667	1671	rBV2	163463	200811	5.08%	0.587%
28	11.963	1676	1679	1682	rBV	104045	105997	2.68%	0.310%
29	12.092	1697	1701	1706	rVB2	176440	206847	5.23%	0.605%
30	12.151	1709	1711	1713	rBV	46721	43829	1.11%	0.128%
31	12.569	1778	1782	1785	rBV	879145	727070	18.38%	2.126%
32	12.616	1785	1790	1795	rBV2	52596	52450	1.33%	0.153%
33	12.663	1795	1798	1800	rBV4	53622	54400	1.38%	0.159%
34	12.798	1813	1821	1824	rBV2	560169	727497	18.40%	2.128%
35	12.851	1826	1830	1836	rVB	30949	45403	1.15%	0.133%
36	12.951	1843	1847	1850	rBV	4212127	3745481	94.71%	10.954%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102623\
Data File : BF135961.D
Acq On : 26 Oct 2023 14:00
Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

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-BF102523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.021	1853	1859	1862	rBV2	28932	45848	1.16%	0.134%
38	13.127	1874	1877	1881	rVB	91394	85601	2.16%	0.250%
39	13.198	1885	1889	1891	rBV	82068	76387	1.93%	0.223%
40	13.227	1891	1894	1897	rBV	45685	48236	1.22%	0.141%
41	13.751	1979	1983	1986	rVB2	47491	50711	1.28%	0.148%
42	14.004	2018	2026	2028	rBV2	1165341	1282288	32.42%	3.750%
43	14.027	2028	2030	2033	rVB	233625	183823	4.65%	0.538%
44	15.051	2199	2204	2207	rBV	176163	266754	6.74%	0.780%
45	15.162	2220	2223	2227	rVB2	38736	43279	1.09%	0.127%
46	15.357	2251	2256	2262	rVB	103797	130953	3.31%	0.383%
47	15.421	2262	2267	2272	rBV	120221	155032	3.92%	0.453%
48	15.486	2272	2278	2288	rBV	903906	1124876	28.44%	3.290%
49	16.980	2527	2532	2541	rVB3	52615	114279	2.89%	0.334%
50	17.427	2604	2608	2614	rBV	41252	76440	1.93%	0.224%

Sum of corrected areas: 34193396

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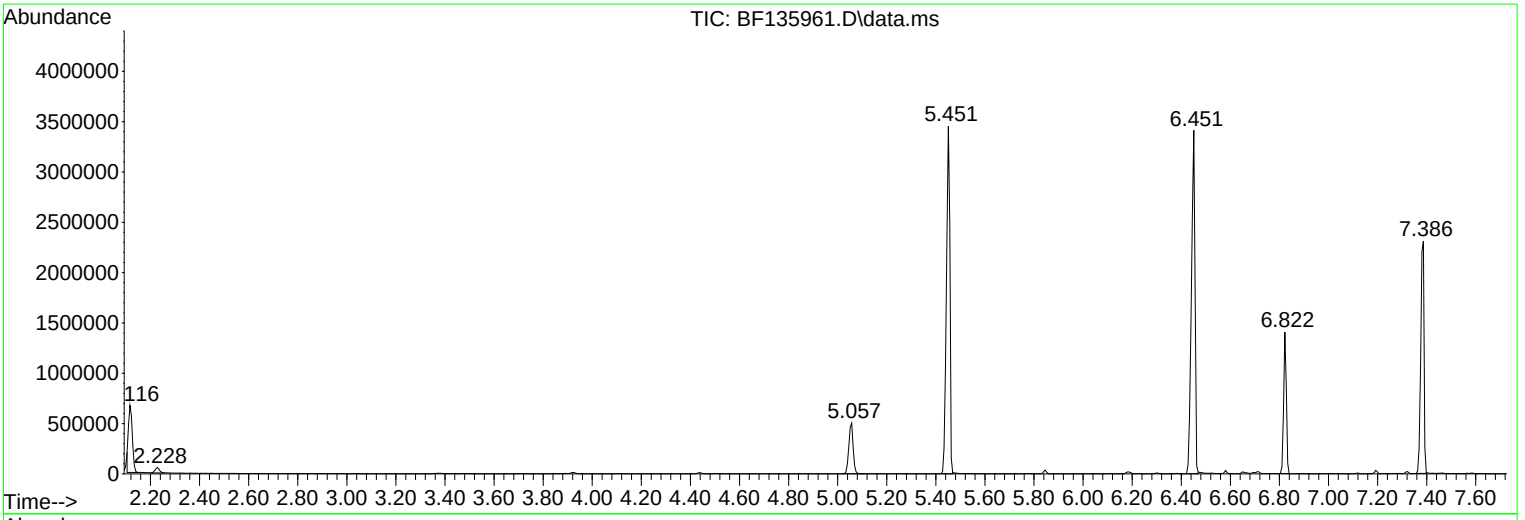
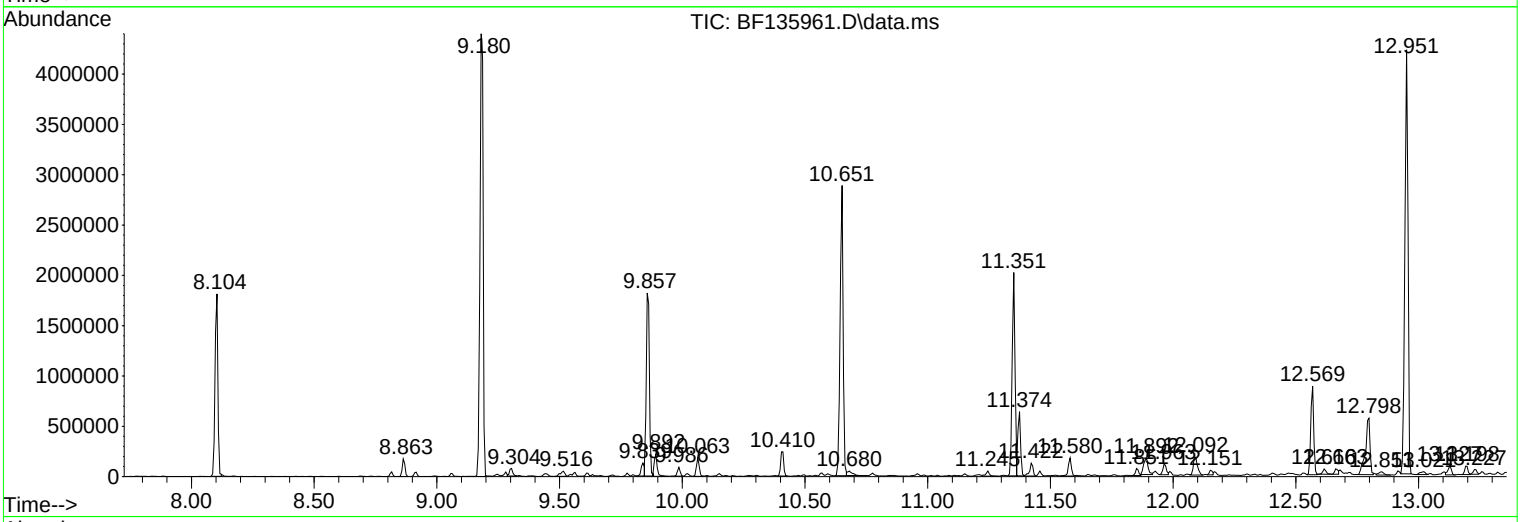
Misc :
ALS Vial : 5 Sample Multiplier: 1

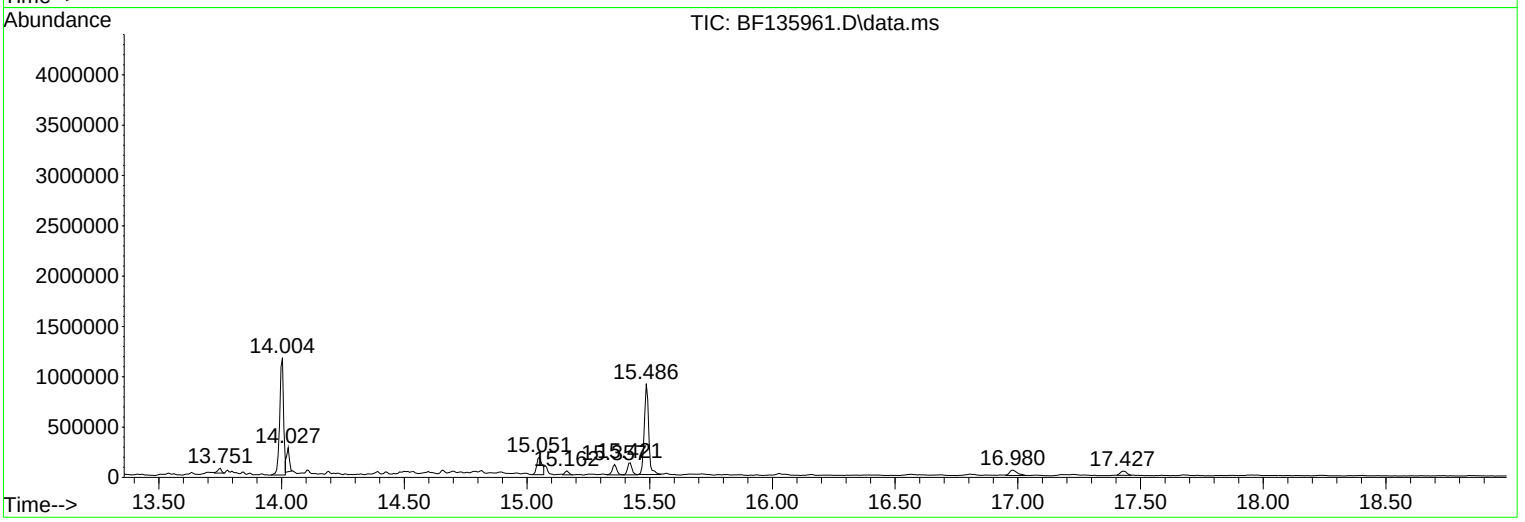
Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.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\BF102623\
Data File : BF135961.D
Acq On : 26 Oct 2023 14:00
Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

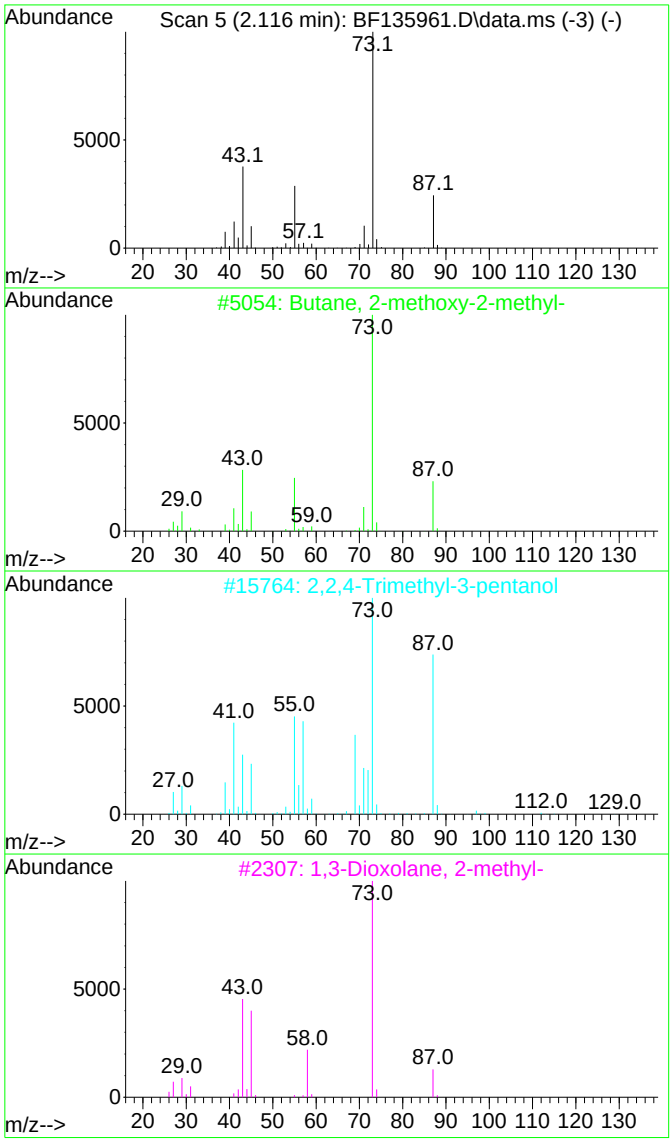
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

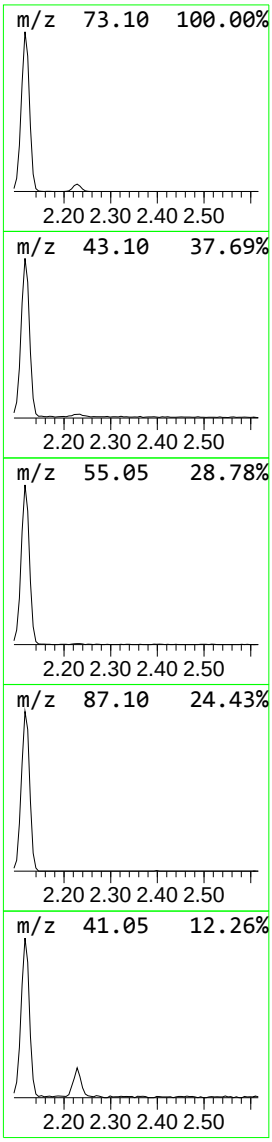
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	13.53 ng	723888	1,4-Dichlorobenzene-d4	6.822

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102623\
Data File : BF135961.D
Acq On : 26 Oct 2023 14:00
Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

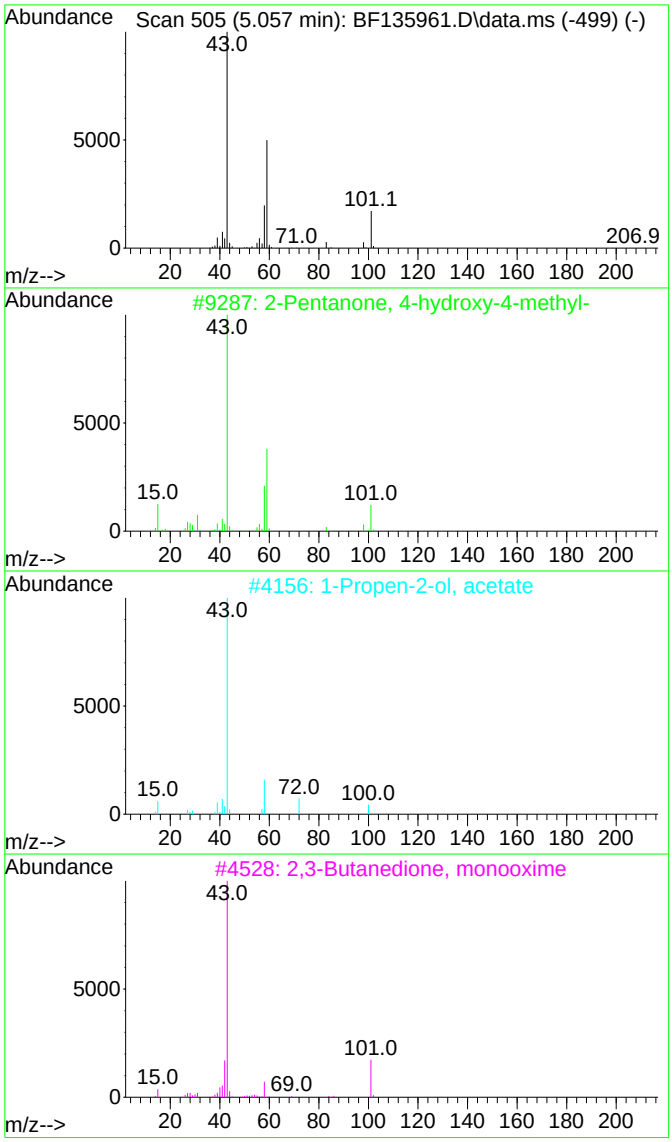
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

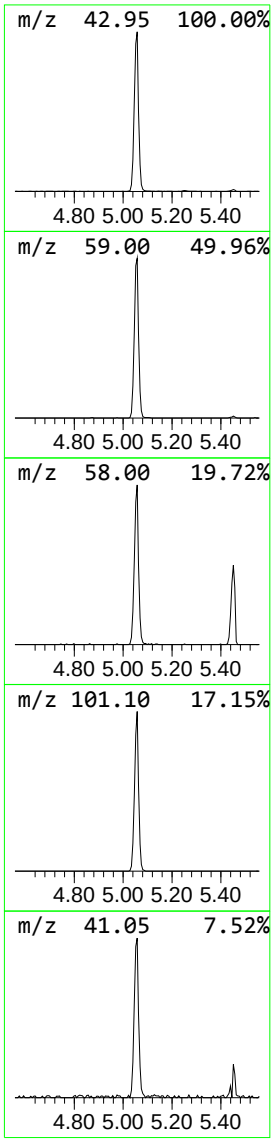
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	11.46 ng	613580	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Acetone	58	C3H6O	000067-64-1	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102623\
Data File : BF135961.D
Acq On : 26 Oct 2023 14:00
Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

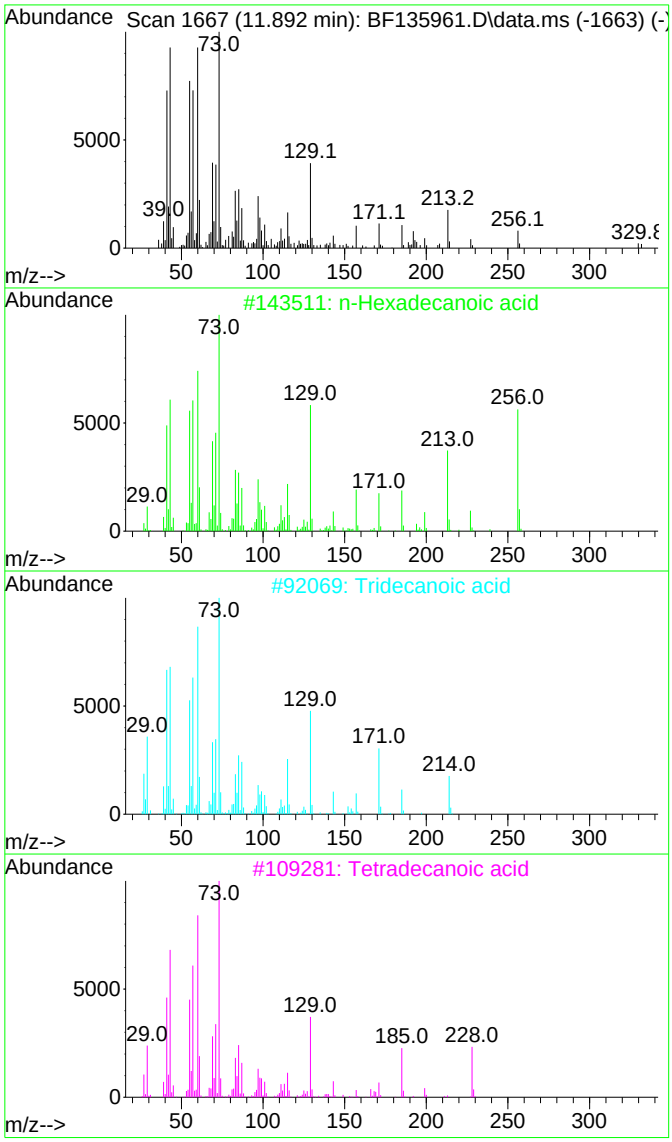
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

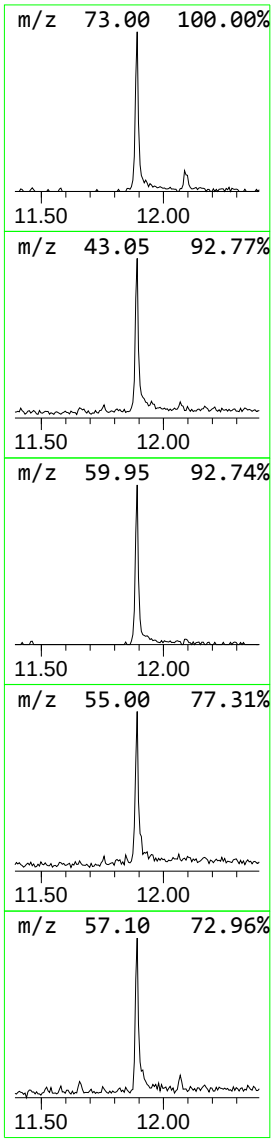
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.41 ng	200811	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	91
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102623\
Data File : BF135961.D
Acq On : 26 Oct 2023 14:00
Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

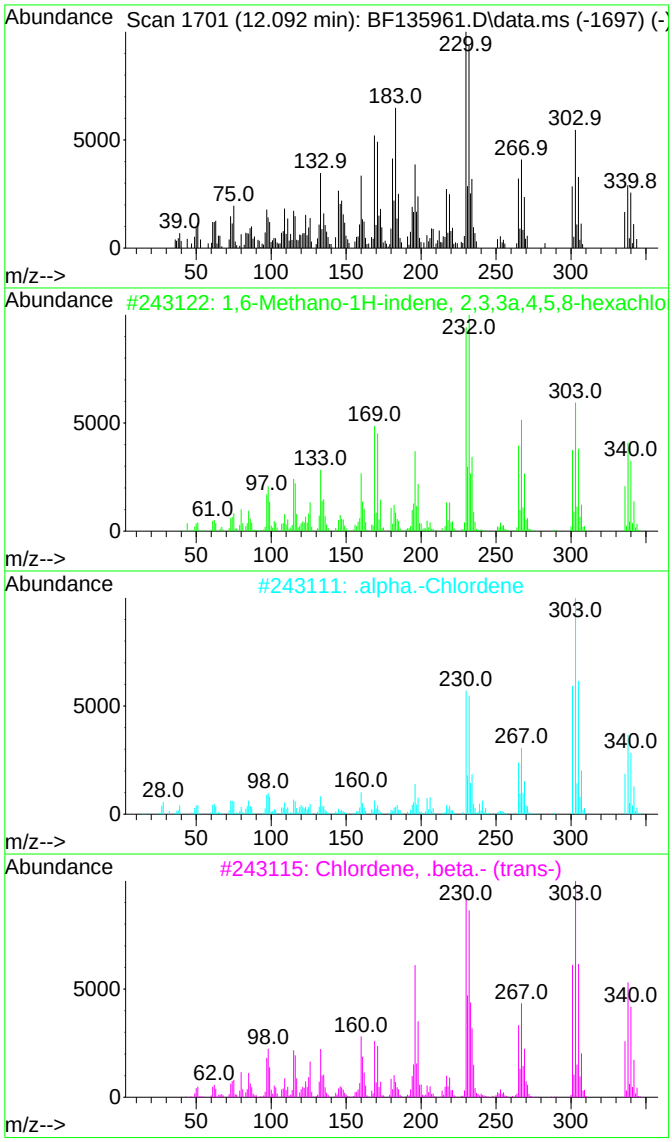
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

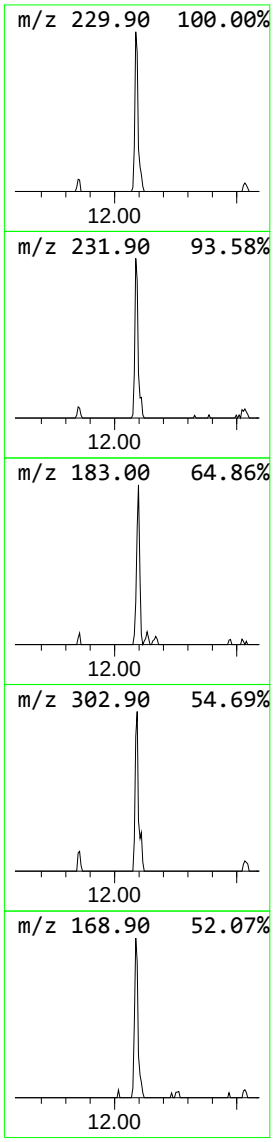
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,6-Methano-1H-indene, 2,3,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	2.49 ng	206847	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Methano-1H-indene, 2,3,3a,4,...	336	C10H6Cl6	056641-38-4	99
2	.alpha.-Chlordene	336	C10H6Cl6	056534-02-2	99
3	Chlordene, .beta.- (trans-)	336	C10H6Cl6	1000378-50-4	90
4	1-Perchloroethenyl-4-ethynylbenzene	230	C10H5Cl3	1000283-76-9	81
5	3-Bromo-6-chloro-1H-pyrrolo[2,3-...	230	C7H4BrClN2	1190321-08-4	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102623\
Data File : BF135961.D
Acq On : 26 Oct 2023 14:00
Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

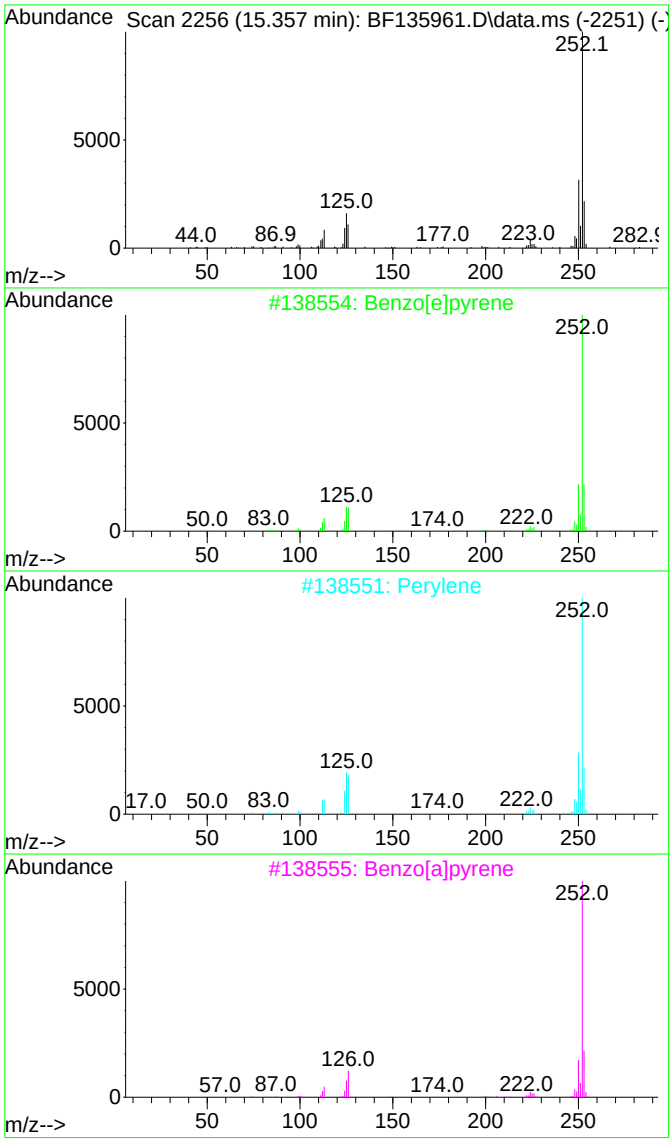
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

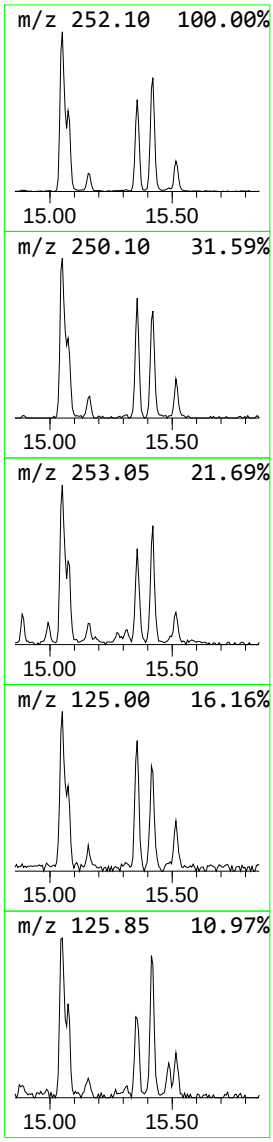
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.357	2.33 ng	130953	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





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Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

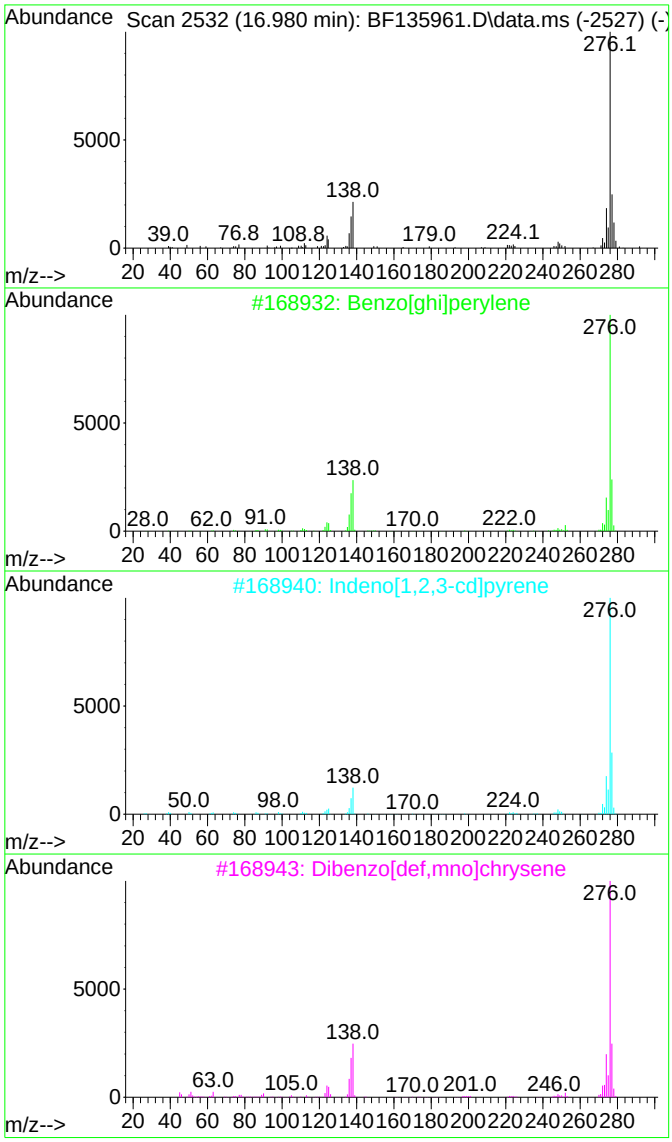
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

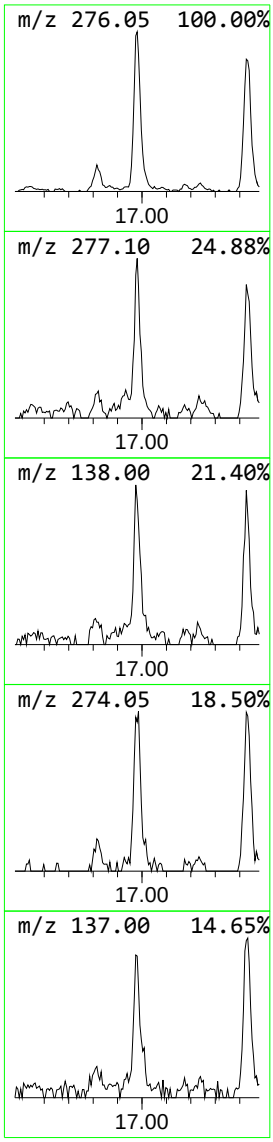
****

Peak Number 6 Dibenzo[def,mno]chrysene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.980	2.03 ng	114279	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[ghi]perylene	276	C22H12	000191-24-2	95
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	93
3	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	91
4	1H-Indol-6-ylamine, 2TMS derivative	276	C14H24N2Si2	1000484-86-0	53
5	12H-Benzothieno[2,3-d]pyrido[1,2...	276	C14H16N2S2	102254-63-7	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102623\
Data File : BF135961.D
Acq On : 26 Oct 2023 14:00
Operator : CG\JU
Sample : 05015-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.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...	2.116	13.5	ng	723888	1	6.822	1070430	20.0
2-Pentanone, 4-...	5.057	11.5	ng	613580	1	6.822	1070430	20.0
n-Hexadecanoic ...	11.892	2.4	ng	200811	4	11.351	1664220	20.0
1,6-Methano-1H-...	12.092	2.5	ng	206847	4	11.351	1664220	20.0
Benzo[e]pyrene	15.357	2.3	ng	130953	6	15.486	1124880	20.0
Dibenzo[def,mno...	16.980	2.0	ng	114279	6	15.486	1124880	20.0