LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
Acq On : 22 Dec 2022 02:40
Operator : CG\JU
Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N40305

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-BF122022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131767.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	15	rVB	432412	549907	22.62%	2.160%
2	5.081	503	509	523	rVB	706354	923417	37.98%	3.627%
3	5.481	572	577	580	rBV	2386030	2190542	90.09%	8.604%
4	6.493	744	749	752	rBV	2094440	2263991	93.12%	8.893%
5	6.863	808	812	815	rBV	638644	507182	20.86%	1.992%
6	7.434	903	909	912	rBV	1540277	1449537	59.62%	5.694%
7	7.692	949	953	956	rVB	52439	48866	2.01%	0.192%
8	8.151	1026	1031	1033	rBV	783104	640225	26.33%	2.515%
9	8.175	1033	1035	1038	rVB	98440	76391	3.14%	0.300%
10	8.869	1147	1153	1156	rVB2	46410	42232	1.74%	0.166%
11	9.234	1209	1215	1218	rBV	2981813	2431370	100.00%	9.550%
12	9.916	1325	1331	1334	rBV	931969	765730	31.49%	3.008%
13	9.945	1334	1336	1339	rVB	335822	246927	10.16%	0.970%
14	10.116	1362	1365	1370	rBV	113783	96608	3.97%	0.379%
15	10.463	1420	1424	1428	rBV	207334	163705	6.73%	0.643%
16	10.633	1449	1453	1456	rVB2	98389	99783	4.10%	0.392%
17	10.710	1461	1466	1469	rBV	1868839	1759563	72.37%	6.912%
18	11.263	1554	1560	1563	rBV2	36994	39225	1.61%	0.154%
19	11.304	1563	1567	1572	rVB	58500	53463	2.20%	0.210%
20	11.410	1581	1585	1587	rBV	897390	875978	36.03%	3.441%
21	11.433	1587	1589	1592	rVV	1128839	823637	33.88%	3.235%
22	11.480	1592	1597	1600	rVV	296226	263540	10.84%	1.035%
23	11.516	1600	1603	1609	rVB2	32357	33223	1.37%	0.131%
24	11.639	1616	1624	1631	rBV	173922	146274	6.02%	0.575%
25	11.910	1665	1670	1672	rBV	80495	76252	3.14%	0.300%
26	11.933	1672	1674	1679	rVB	245081	206565	8.50%	0.811%
27	11.986	1680	1683	1686	rVB	42364	34442	1.42%	0.135%
28	12.022	1686	1689	1692	rBV2	185627	181456	7.46%	0.713%
29	12.204	1718	1720	1723	rVB	59268	49048	2.02%	0.193%
30	12.463	1760	1764	1767	rBV2	29307	36581	1.50%	0.144%
31	12.627	1788	1792	1795	rBV	1285730	1031753	42.44%	4.053%
32	12.774	1814	1817	1821	rBV2	28825	30685	1.26%	0.121%
33	12.857	1825	1831	1834	rVV	920064	996917	41.00%	3.916%
34	12.904	1836	1839	1845	rVB2	46141	51270	2.11%	0.201%
35	12.998	1851	1855	1861	rVB	2168253	2148570	88.37%	8.440%
36	13.074	1863	1868	1871	rVV3	40590	69413	2.85%	0.273%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
Acq On : 22 Dec 2022 02:40
Operator : CG\JU
Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

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-BF122022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.110	1871	1874	1877	rVV	37205	31422	1.29%	0.123%
38	13.157	1879	1882	1884	rVV3	42345	52928	2.18%	0.208%
39	13.186	1884	1887	1890	rVB	160214	152766	6.28%	0.600%
40	13.251	1895	1898	1900	rVV	200498	158000	6.50%	0.621%
41	13.286	1900	1904	1906	rVV2	66389	73510	3.02%	0.289%
42	13.310	1906	1908	1912	rVB	50902	50466	2.08%	0.198%
43	13.410	1923	1925	1929	rBV2	31511	31367	1.29%	0.123%
44	13.669	1966	1969	1972	rBV2	24448	30450	1.25%	0.120%
45	13.804	1988	1992	1995	rBV	51410	54055	2.22%	0.212%
46	13.833	1995	1997	1999	rBV	55943	43246	1.78%	0.170%
47	13.898	2006	2008	2013	rVB2	29868	30360	1.25%	0.119%
48	14.057	2027	2035	2038	rBV2	778230	1036055	42.61%	4.070%
49	14.086	2038	2040	2045	rVV	314391	287481	11.82%	1.129%
50	14.157	2047	2052	2056	rVB2	156779	203985	8.39%	0.801%
51	14.286	2073	2074	2077	rVB	37710	29267	1.20%	0.115%
52	14.410	2085	2095	2097	rBV5	24468	58492	2.41%	0.230%
53	14.445	2097	2101	2104	rVV	47820	52944	2.18%	0.208%
54	14.521	2111	2114	2116	rBV2	31716	40244	1.66%	0.158%
55	14.592	2124	2126	2129	rVB2	55701	45210	1.86%	0.178%
56	15.110	2210	2214	2218	rBV	198120	319460	13.14%	1.255%
57	15.221	2230	2233	2237	rVB	40320	46425	1.91%	0.182%
58	15.427	2263	2268	2274	rVB	107228	155668	6.40%	0.611%
59	15.486	2274	2278	2284	rBV	169428	214221	8.81%	0.841%
60	15.557	2284	2290	2293	rBV	358210	475447	19.55%	1.868%
61	16.880	2504	2515	2523	rBV8	11175	42869	1.76%	0.168%
62	17.057	2539	2545	2555	rVB2	65331	138329	5.69%	0.543%
63	17.239	2570	2576	2581	rBV2	14914	30804	1.27%	0.121%
64	17.509	2614	2622	2632	rBV3	50513	128265	5.28%	0.504%
65	17.756	2658	2664	2671	rBV	18421	40121	1.65%	0.158%

Sum of corrected areas: 25458125

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
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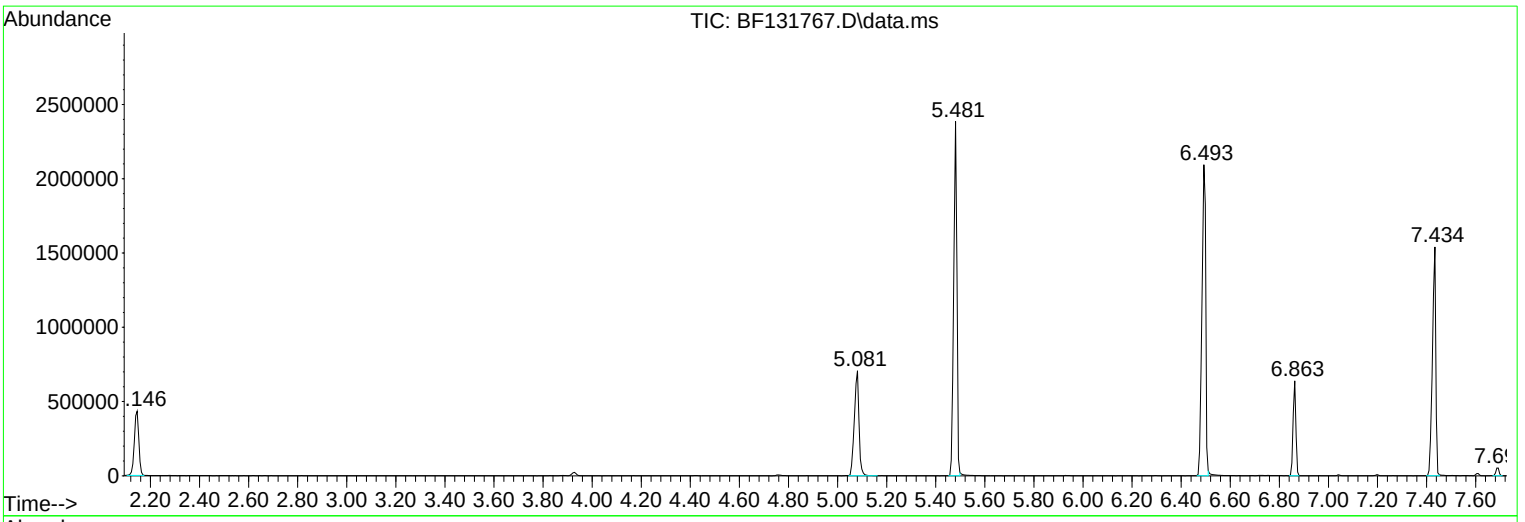
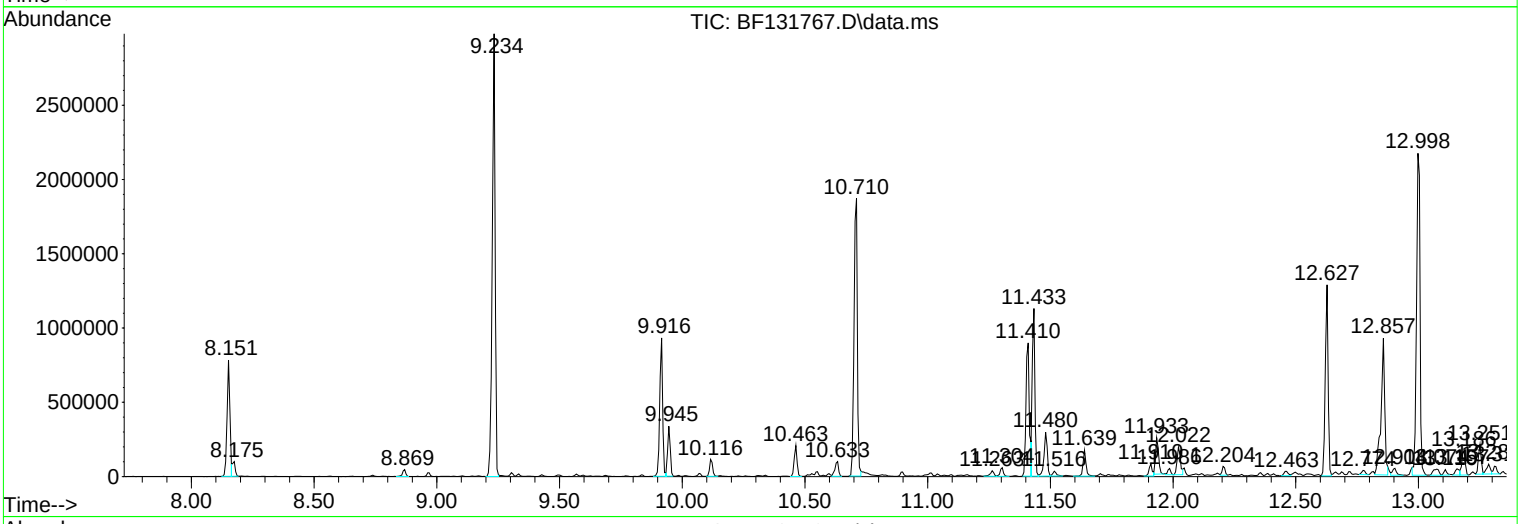
Misc :
ALS Vial : 21 Sample Multiplier: 1

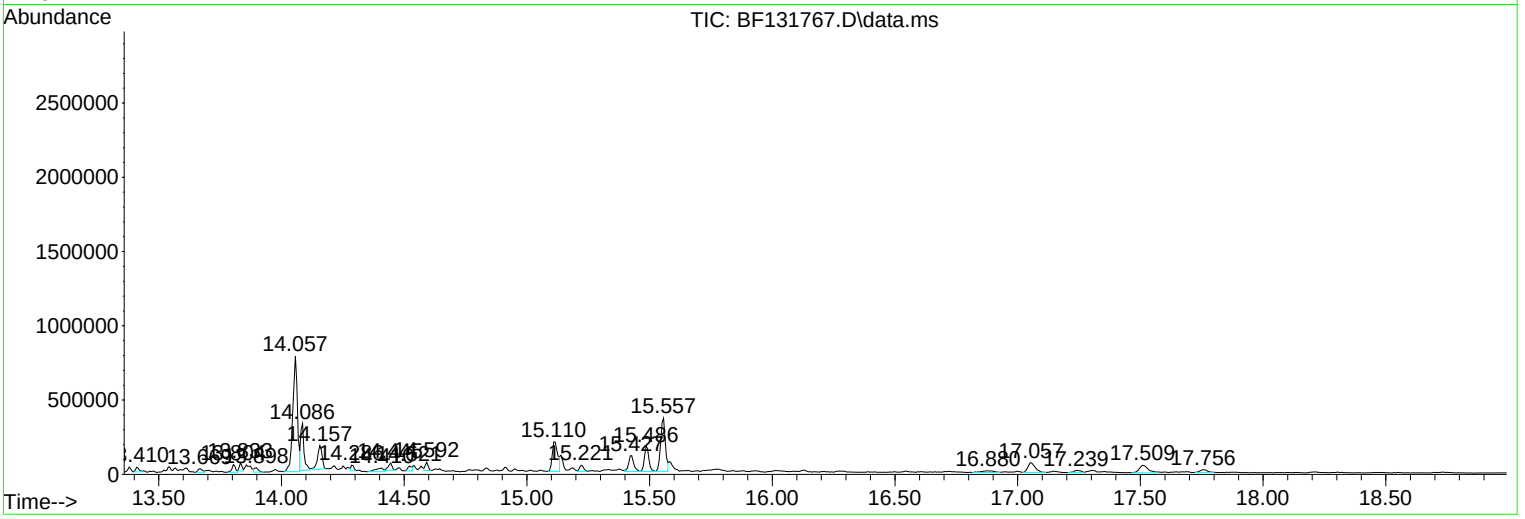
Instrument :
BNA_F
ClientSampleId :
N40305

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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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Data File : BF131767.D
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Instrument :
BNA_F
ClientSampleId :
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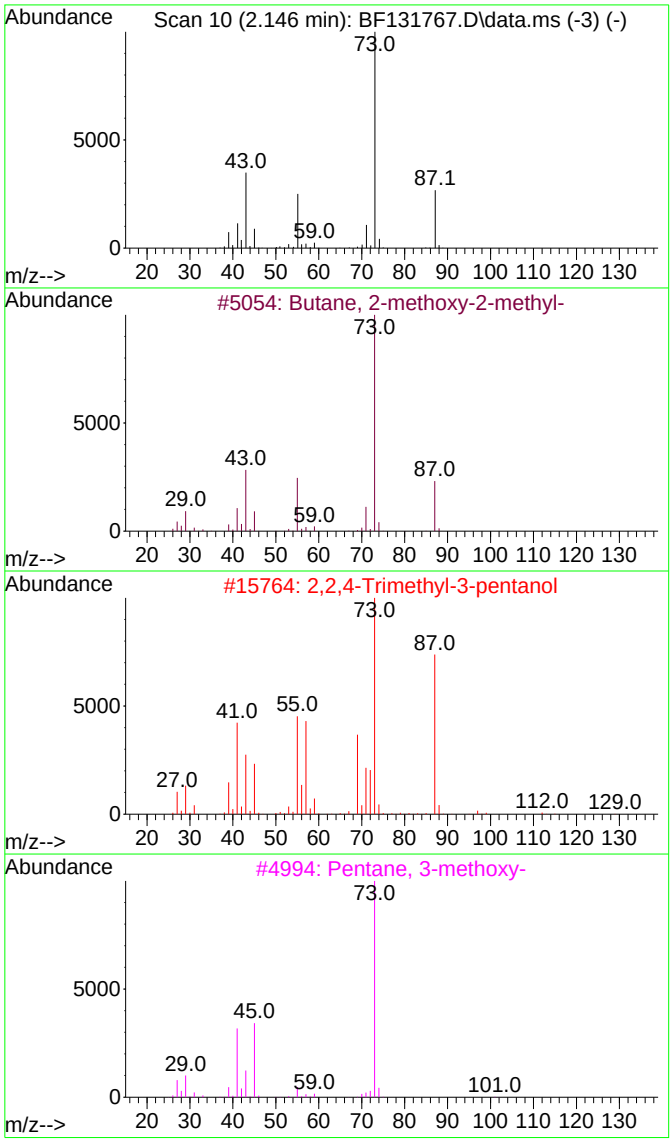
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

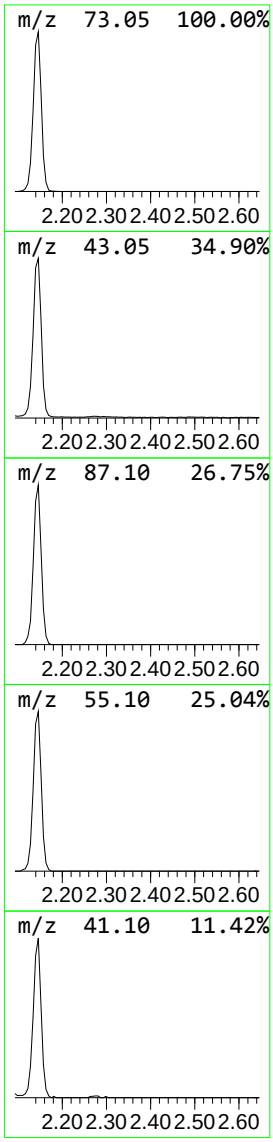
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	21.68 ng	549907	1,4-Dichlorobenzene-d4	6.863

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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
Acq On : 22 Dec 2022 02:40
Operator : CG\JU
Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

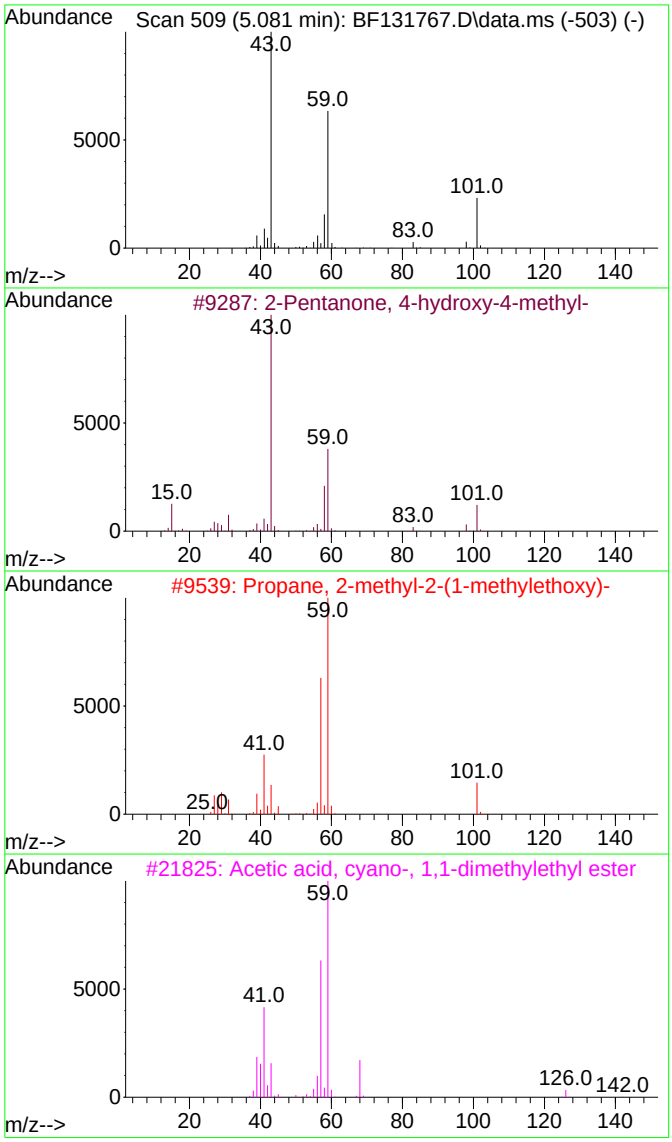
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

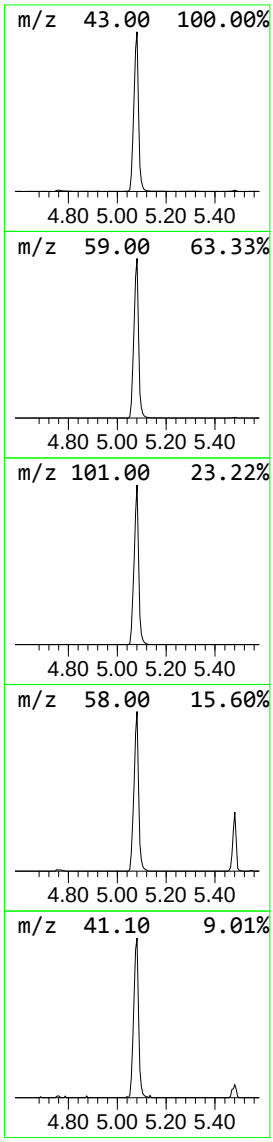
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	36.41 ng	923417	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
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Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

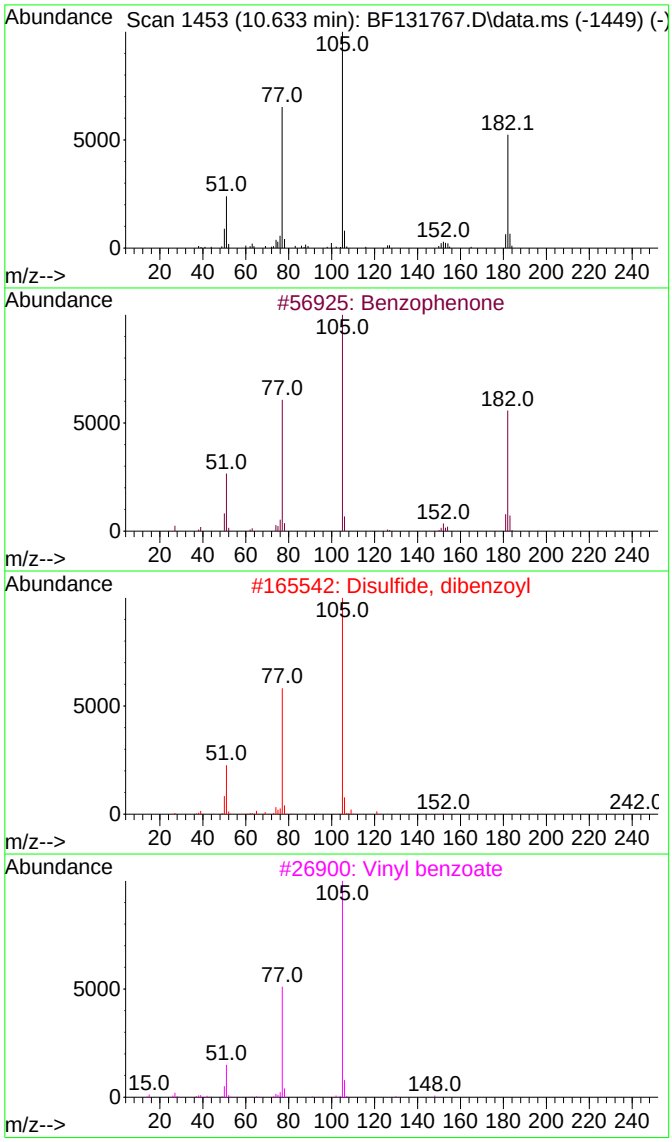
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

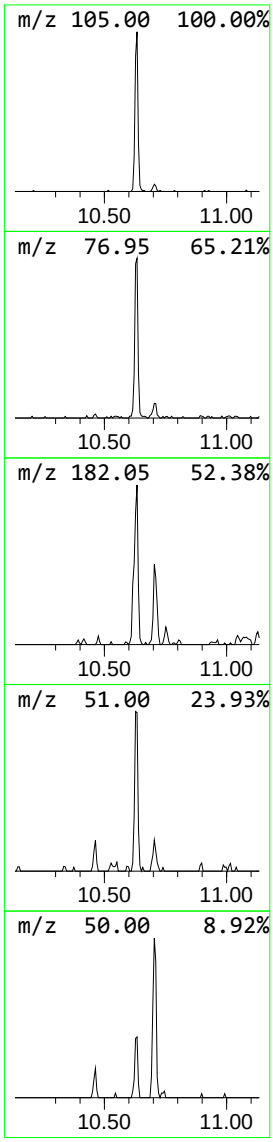
****

Peak Number 3 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	2.61 ng	99783	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47
5	N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
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Operator : CG\JU
Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

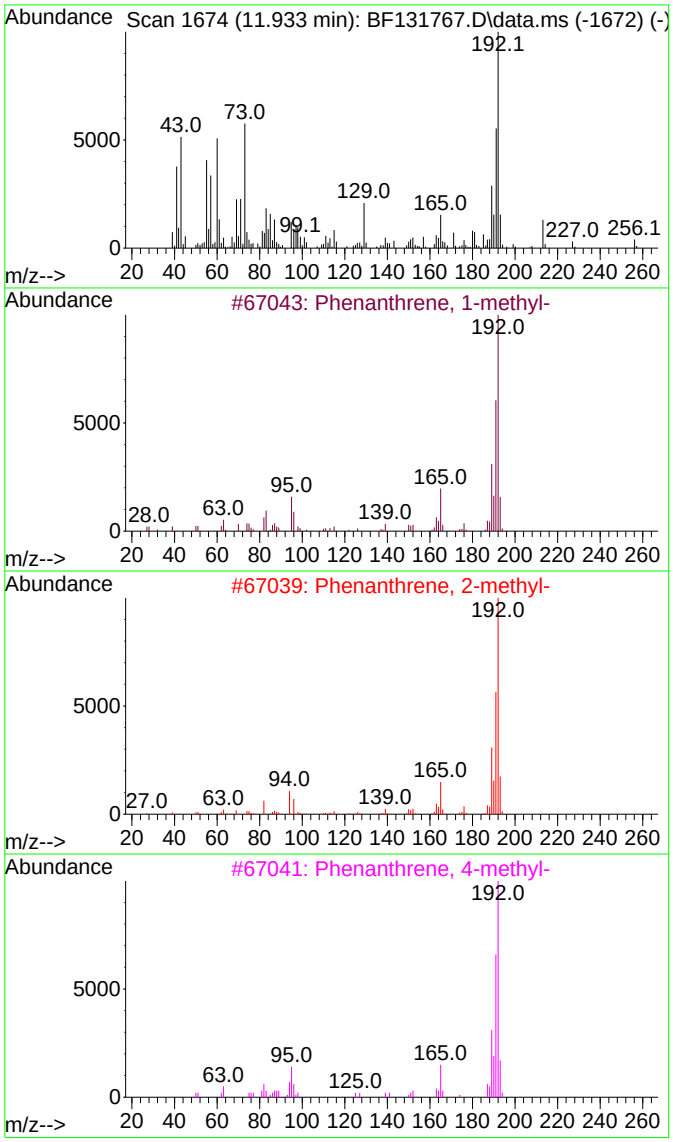
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

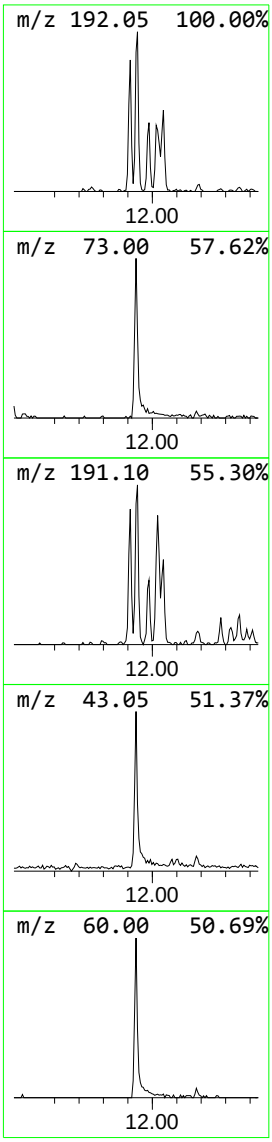
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.72 ng	206565	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
Acq On : 22 Dec 2022 02:40
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Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

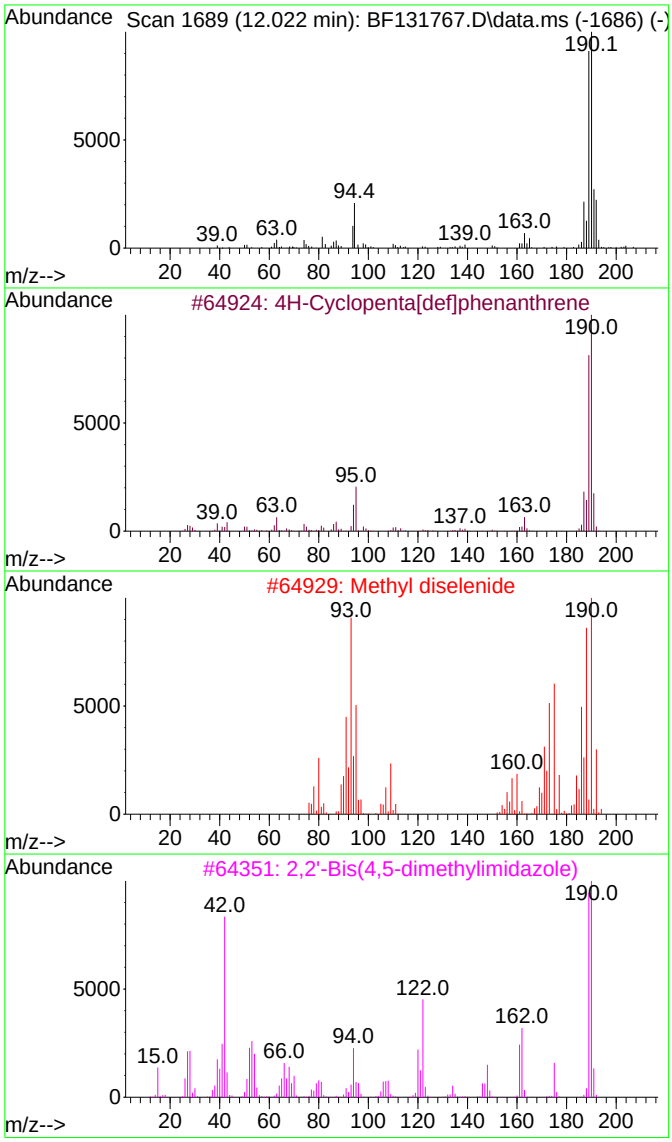
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

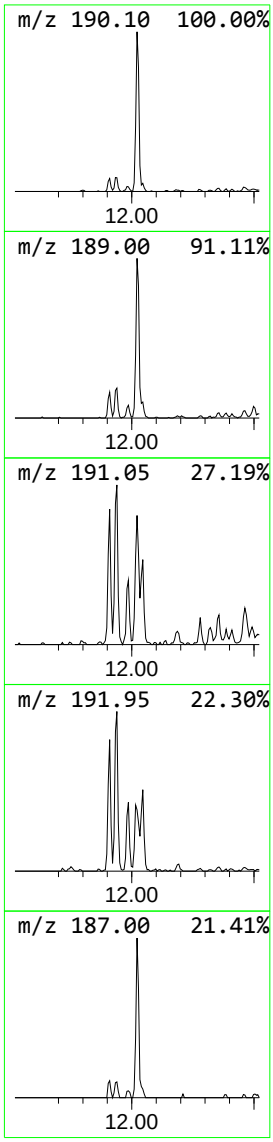
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	4.14 ng	181456	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Methyl diselenide	190	C2H6Se2	007101-31-7	46
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
4	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
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Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

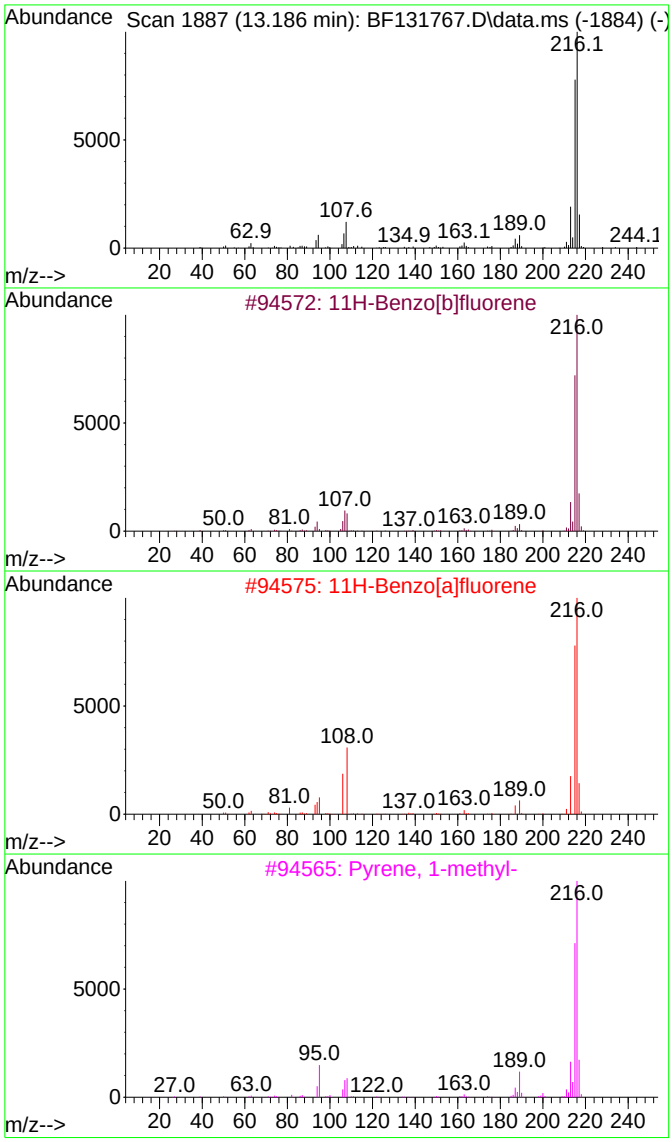
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

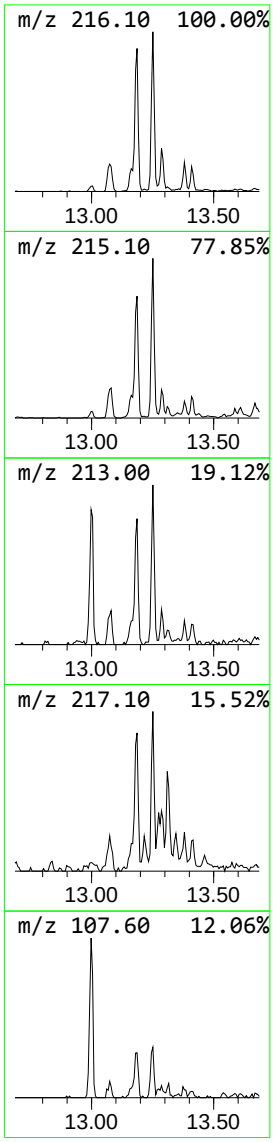
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.186	2.95 ng	152766	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	97
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
Acq On : 22 Dec 2022 02:40
Operator : CG\JU
Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

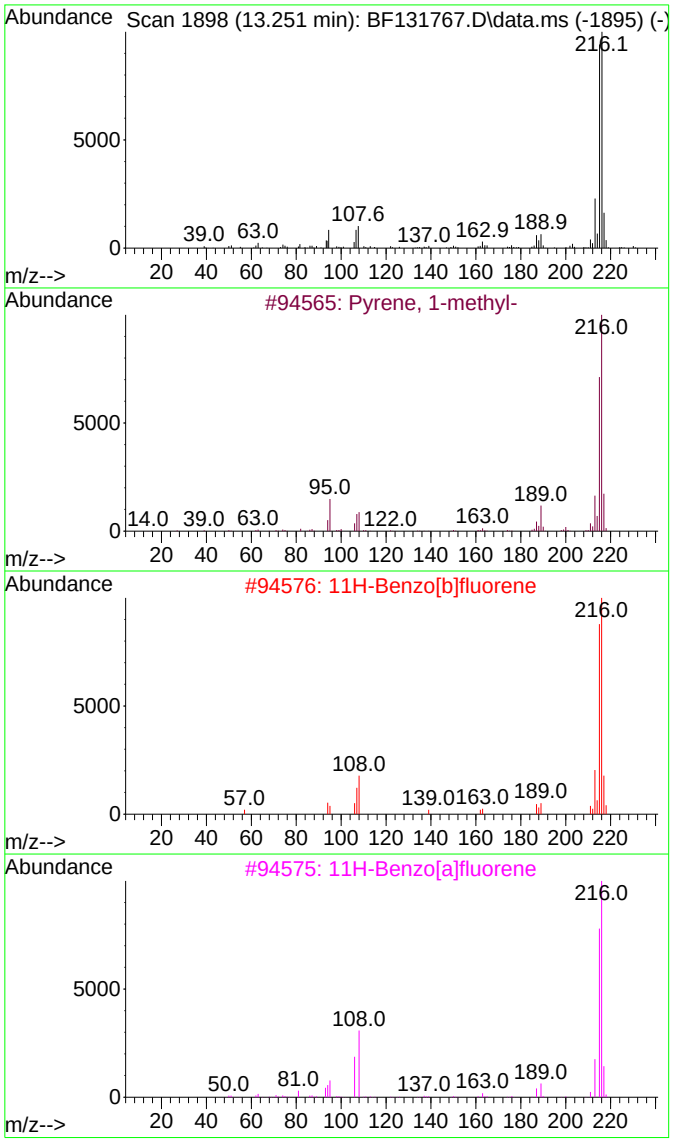
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

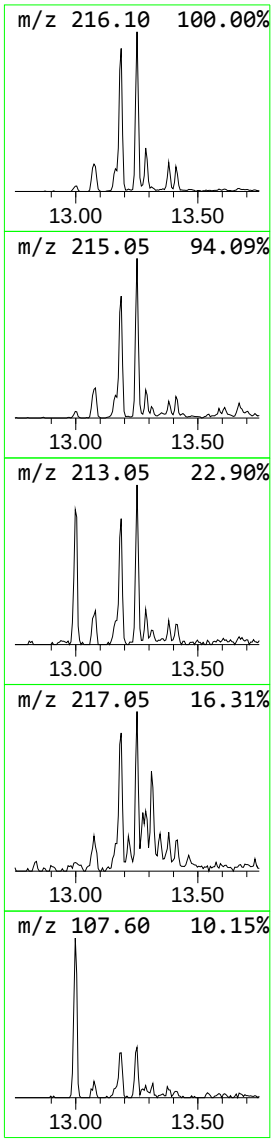
****

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	3.05 ng	158000	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	68





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Acq On : 22 Dec 2022 02:40
Operator : CG\JU
Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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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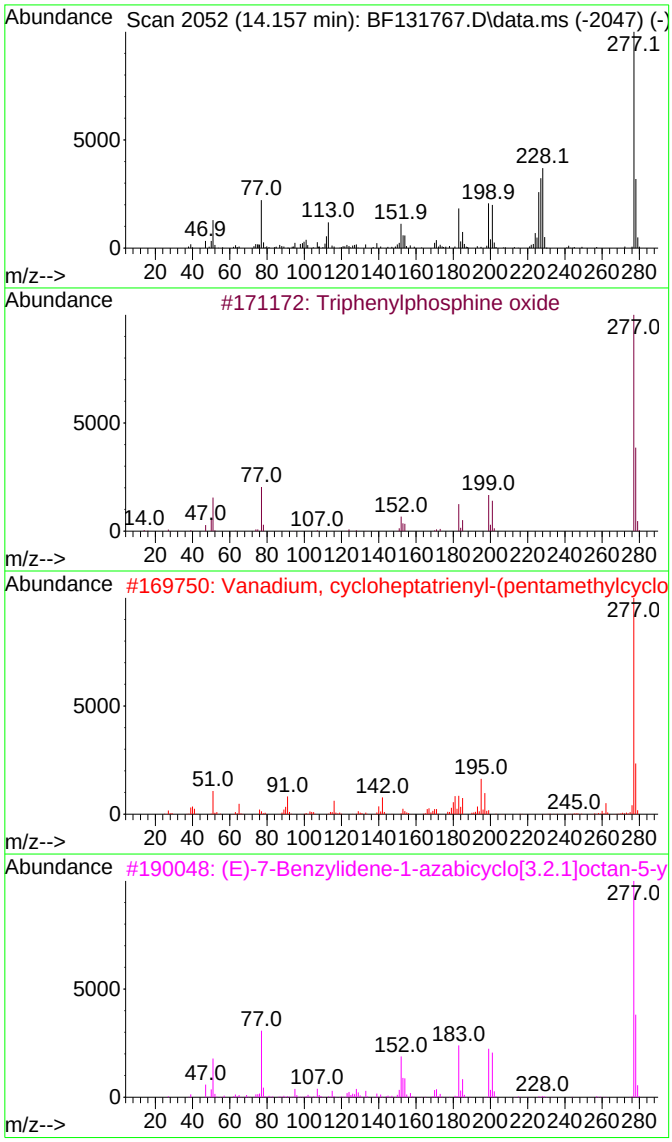
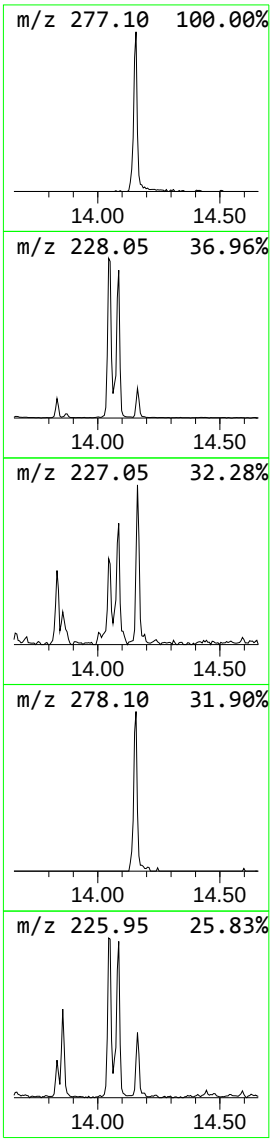
Peak Number 8 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	3.94 ng	203985	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	35
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	27
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	25
5	5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
Acq On : 22 Dec 2022 02:40
Operator : CG\JU
Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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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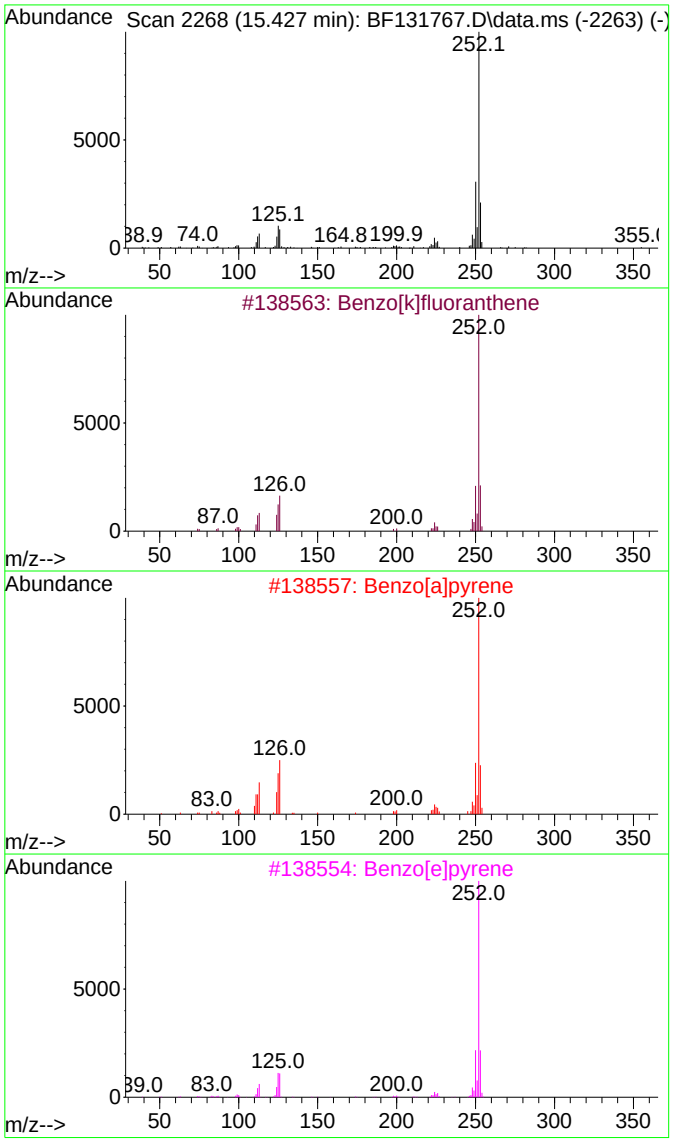
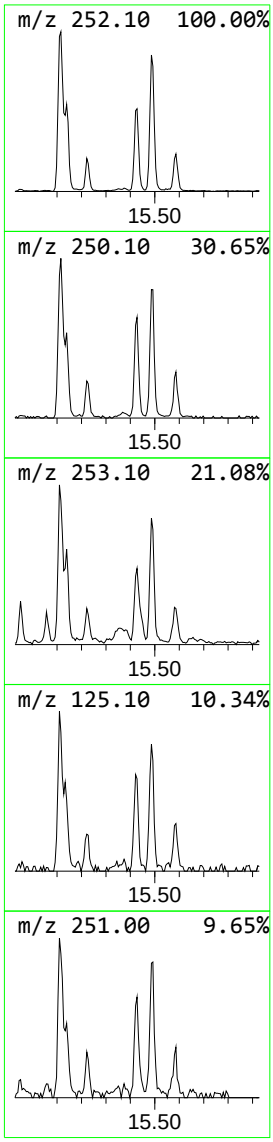
Peak Number 9 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	6.55 ng	155668	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[e]pyrene	252	C20H12	000192-97-2	95
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131767.D
Acq On : 22 Dec 2022 02:40
Operator : CG\JU
Sample : N6161-08
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N40305

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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...	2.146	21.7	ng	549907	1	6.863	507182	20.0
2-Pentanone, 4-...	5.081	36.4	ng	923417	1	6.863	507182	20.0
Benzophenone	10.633	2.6	ng	99783	3	9.916	765730	20.0
Phenanthrene, 1...	11.933	4.7	ng	206565	4	11.410	875978	20.0
4H-Cyclopenta[d...	12.022	4.1	ng	181456	4	11.410	875978	20.0
11H-Benzo[b]flu...	13.186	3.0	ng	152766	5	14.057	1036060	20.0
Pyrene, 1-methyl-	13.251	3.0	ng	158000	5	14.057	1036060	20.0
Triphenylphosph...	14.157	3.9	ng	203985	5	14.057	1036060	20.0
Benzo[e]pyrene	15.427	6.5	ng	155668	6	15.557	475447	20.0